

FIG. 1(a)

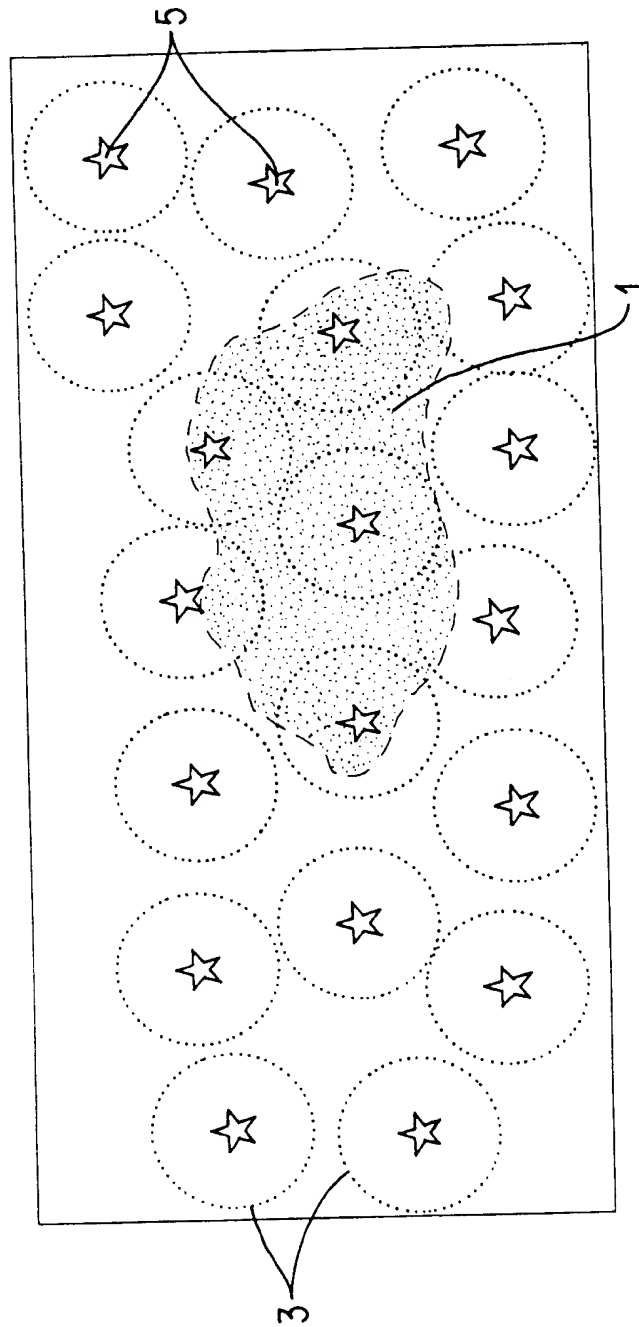


FIG. 1(b)

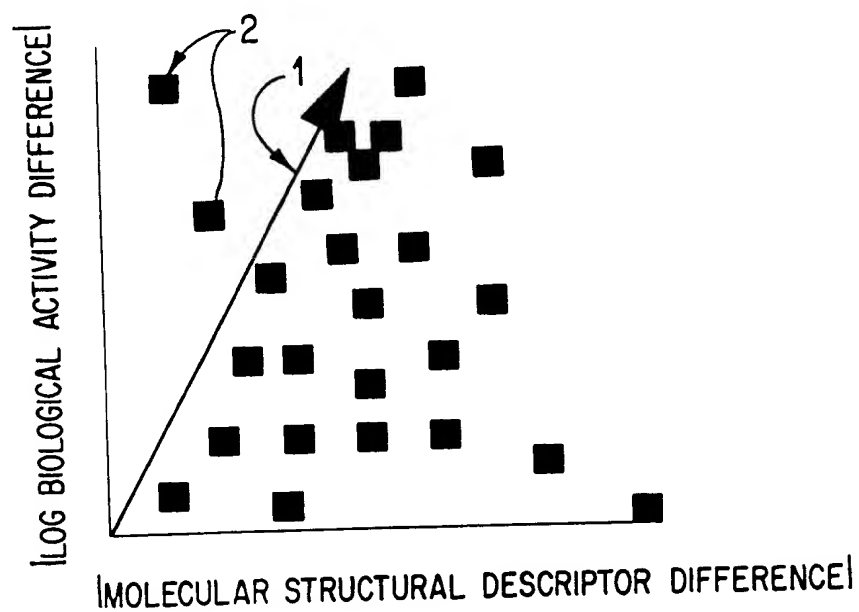


FIG. 2

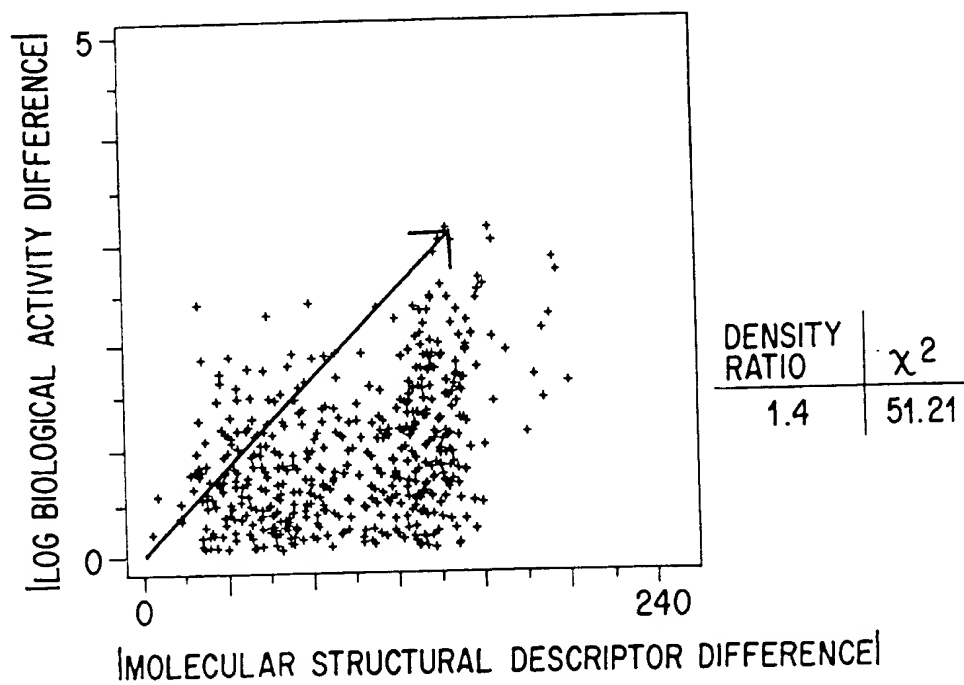
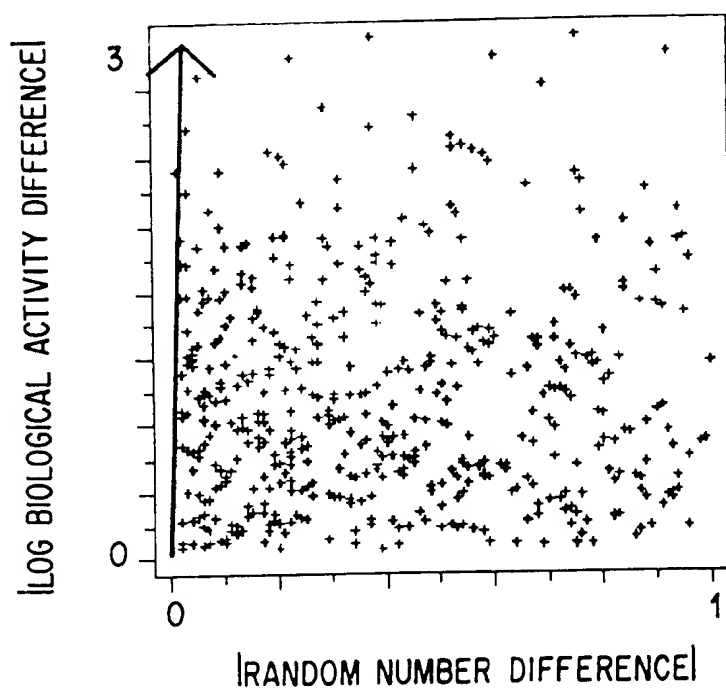
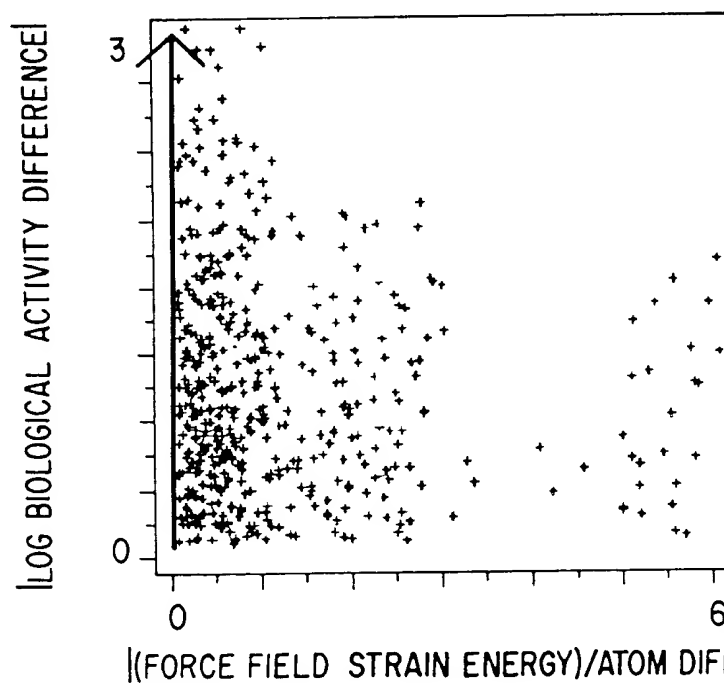


FIG. 3



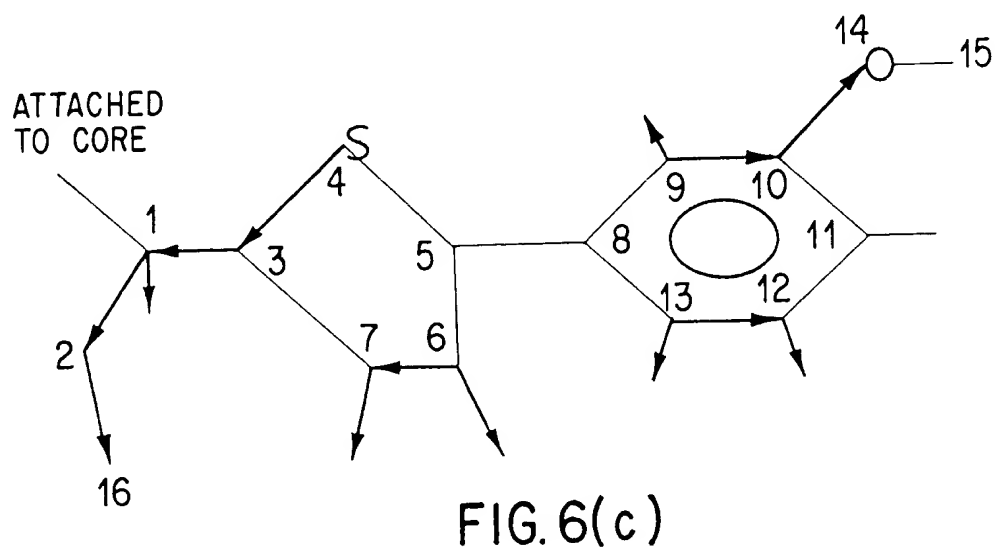
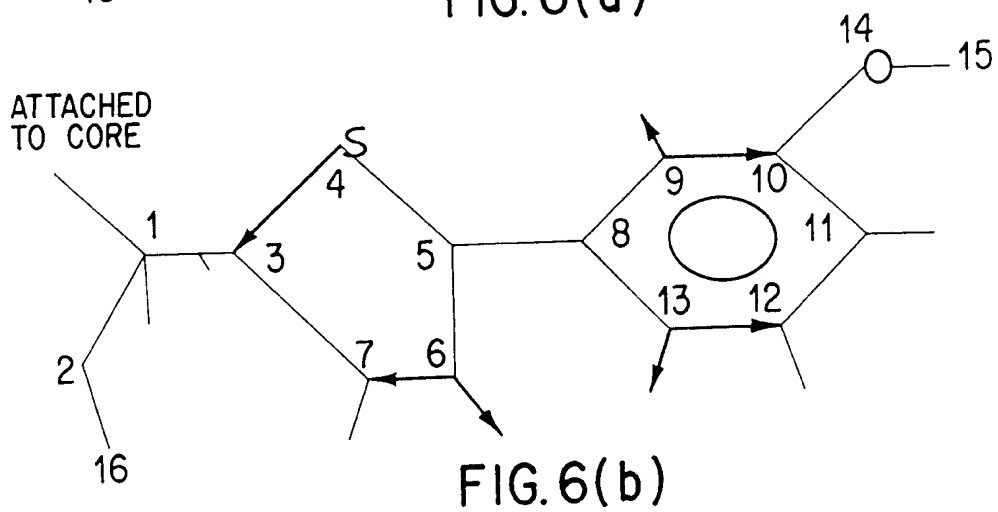
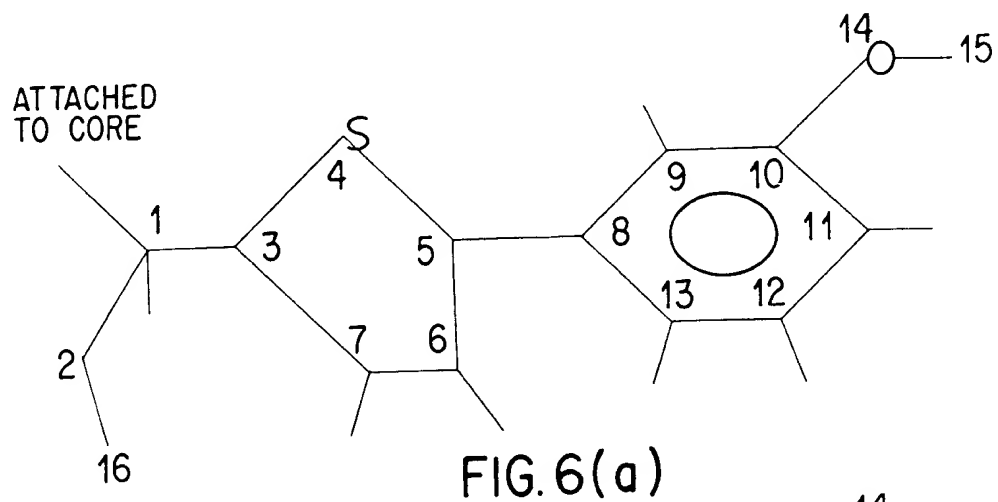
DENSITY RATIO	χ^2
1.00	0.00

FIG. 4



DENSITY RATIO	χ^2
0.96	0.46

FIG. 5



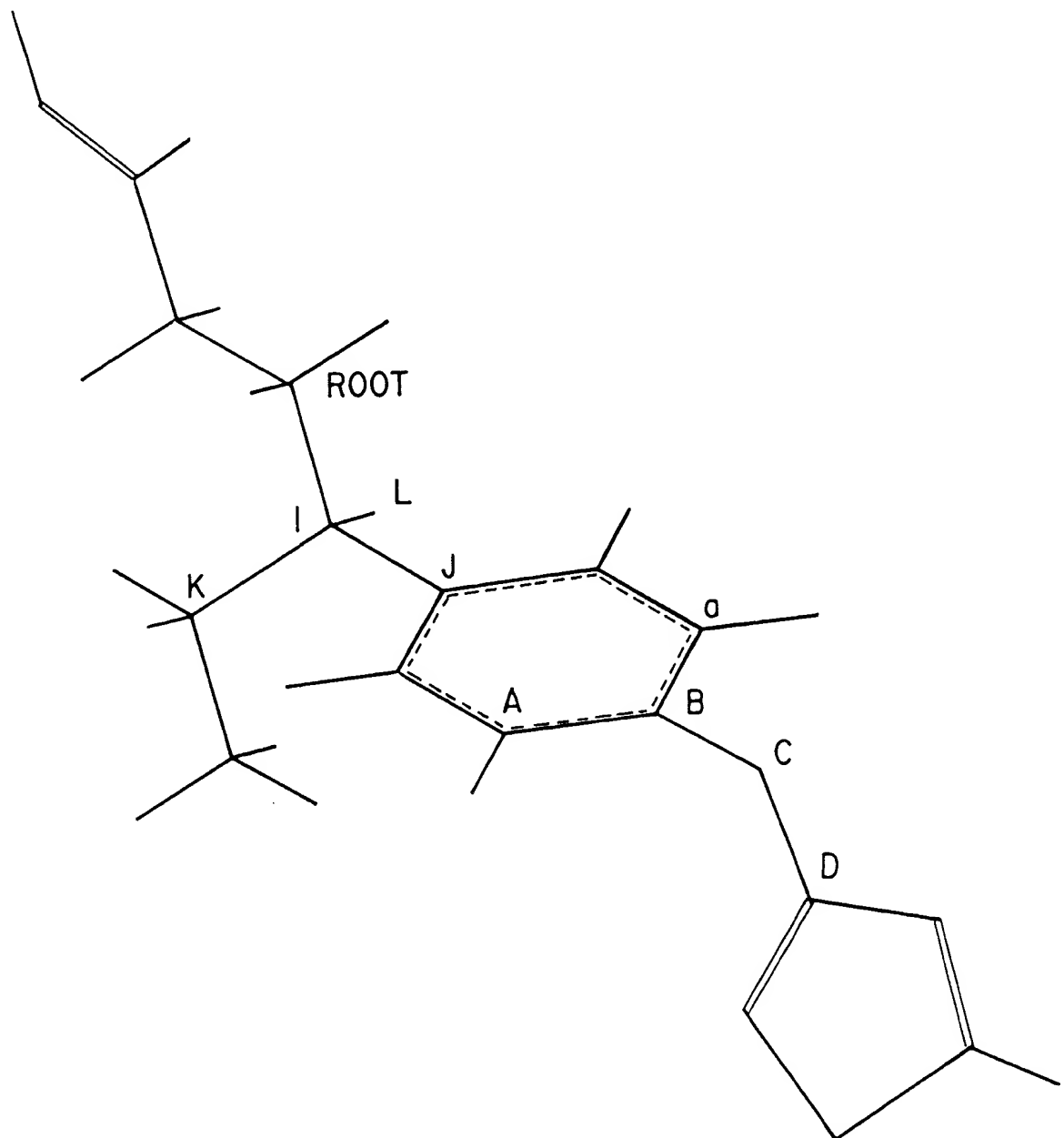


FIG. 6(d)

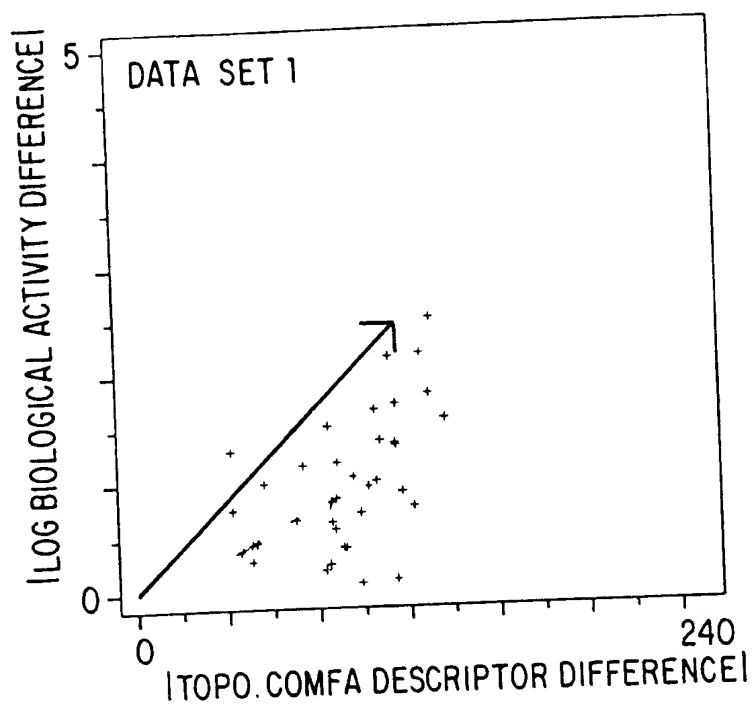


FIG.7(a)

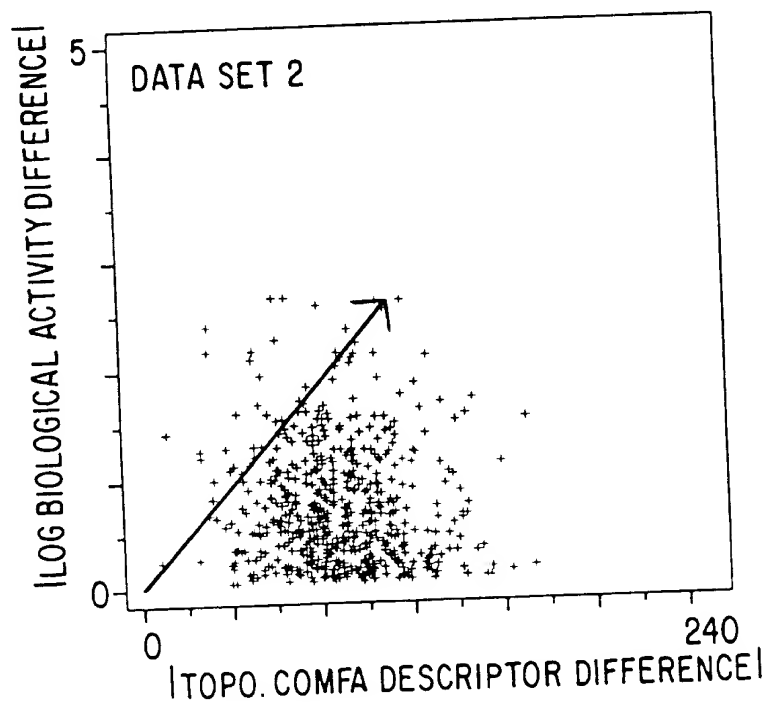


FIG.7(b)

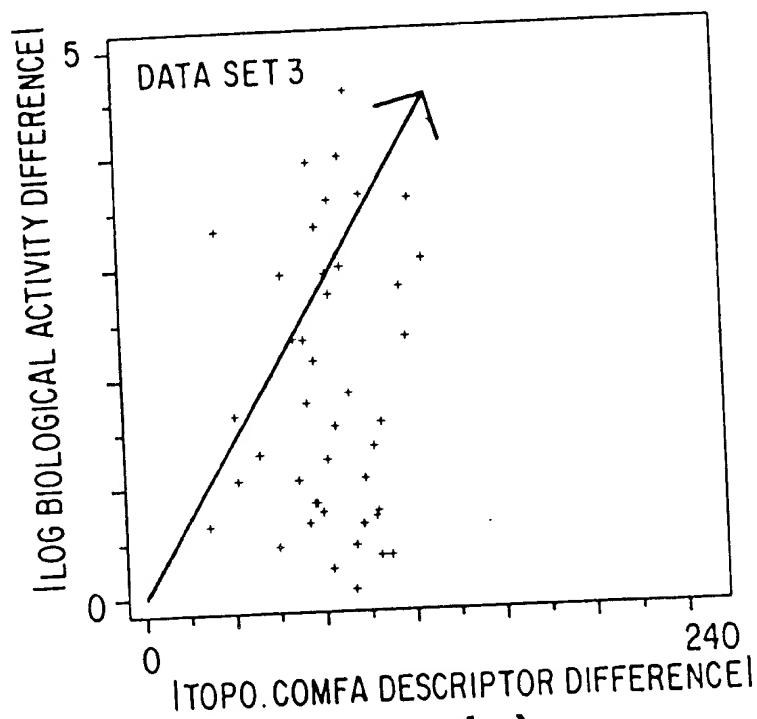


FIG. 7(c)

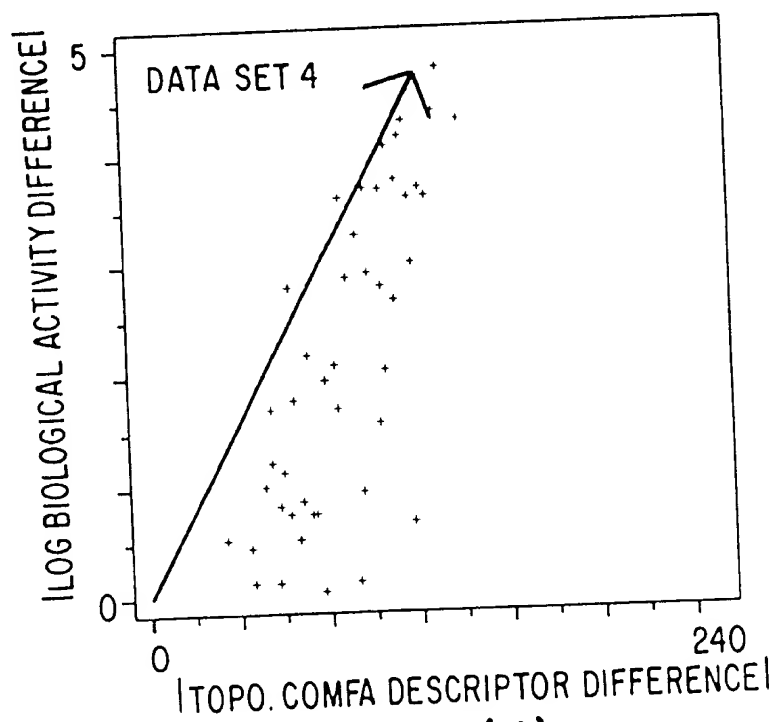


FIG. 7(d)

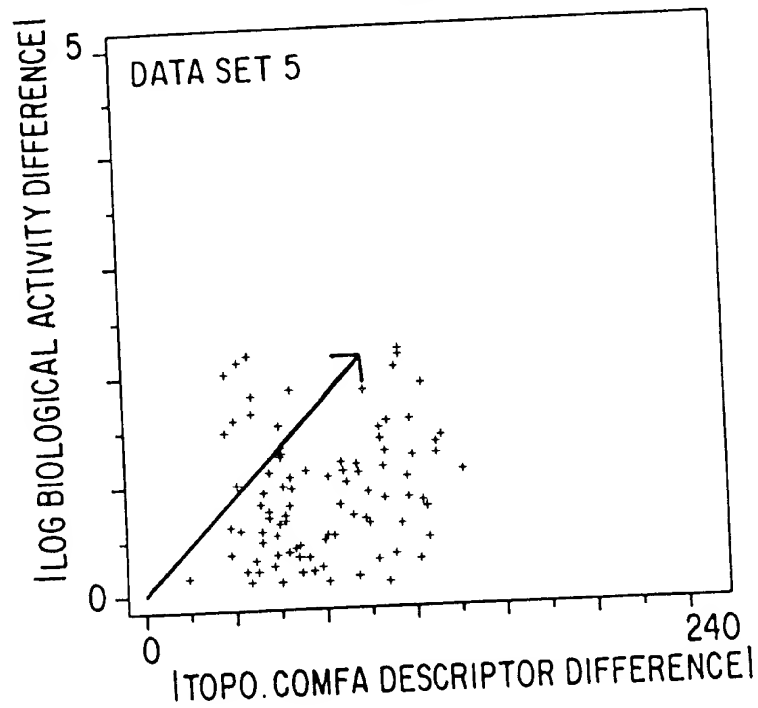


FIG.7(e)

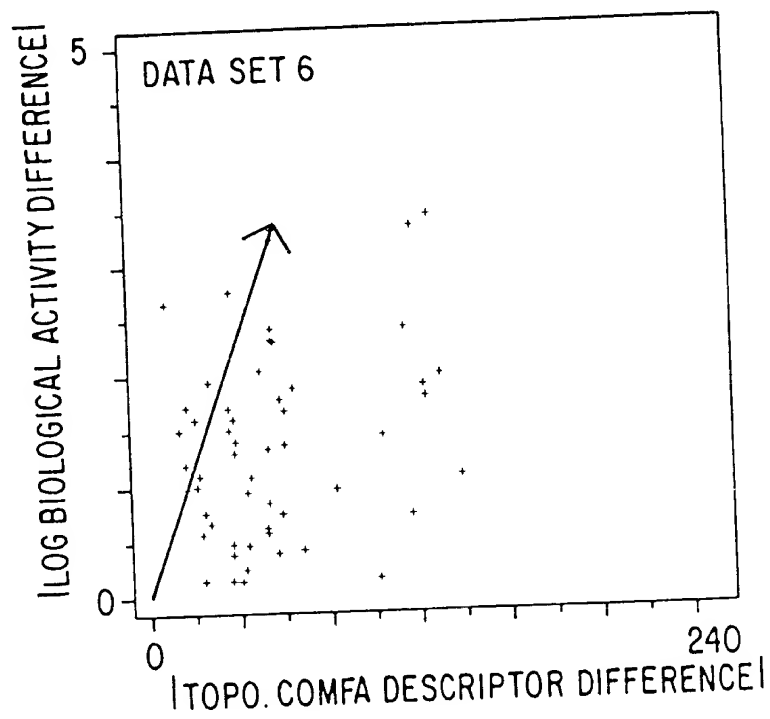


FIG.7(f)

10/44

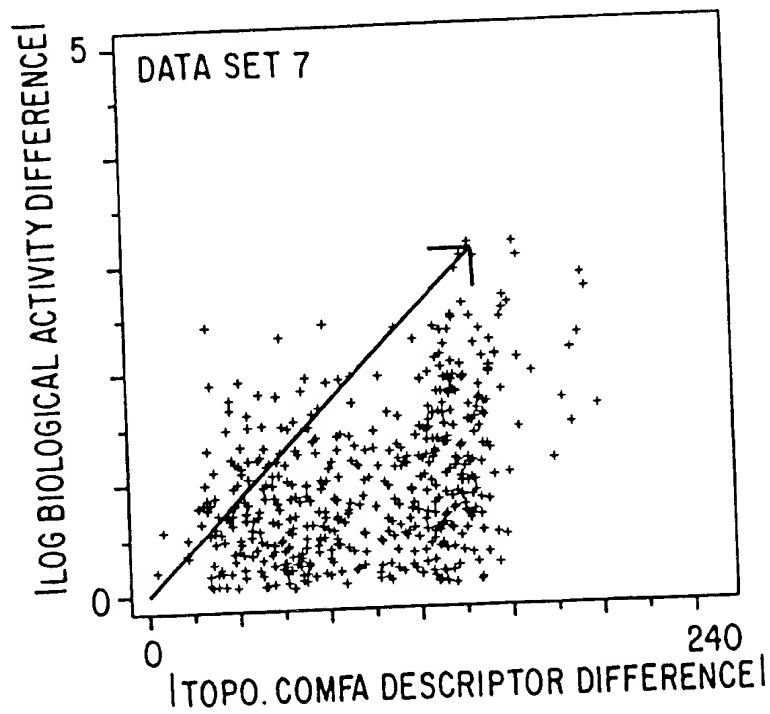


FIG.7(g)

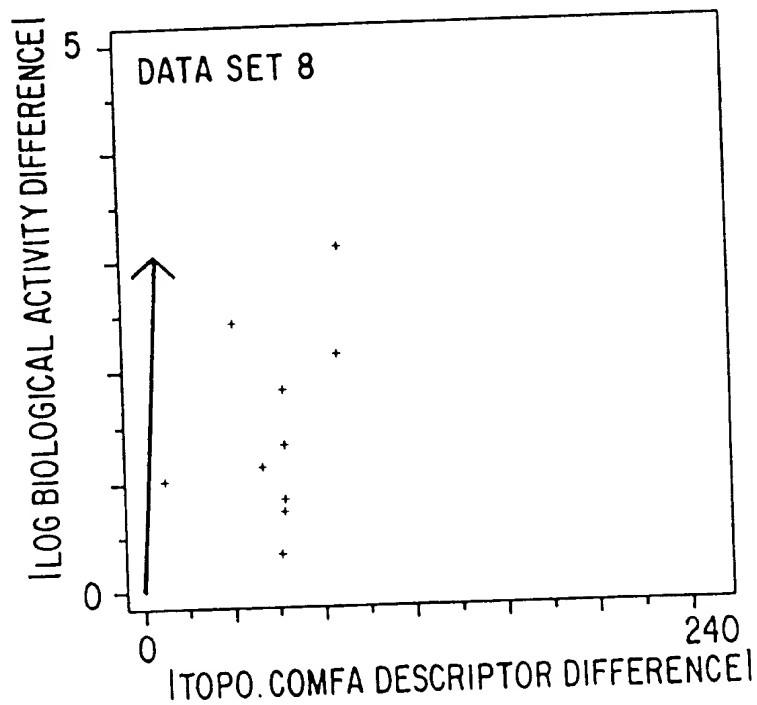


FIG.7(h)

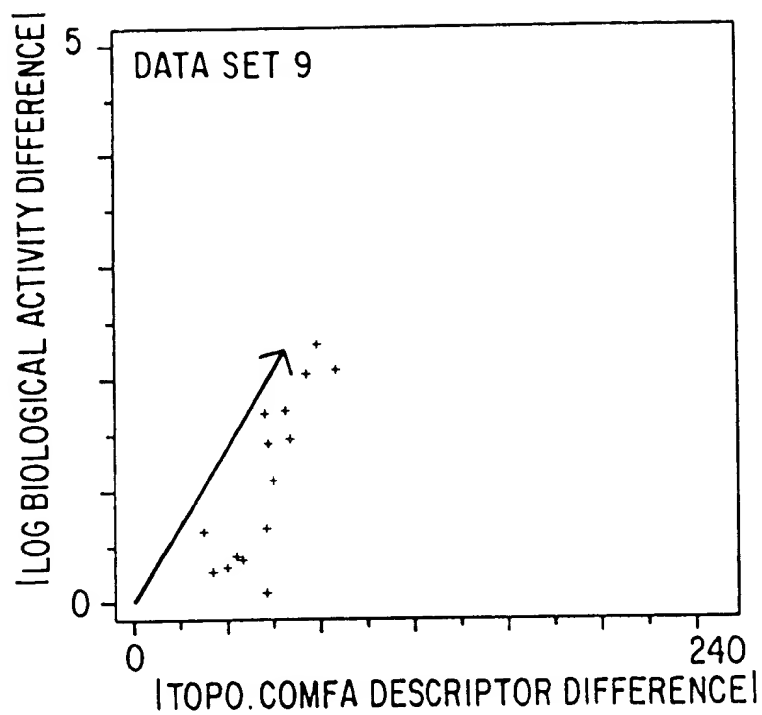


FIG.7(i)

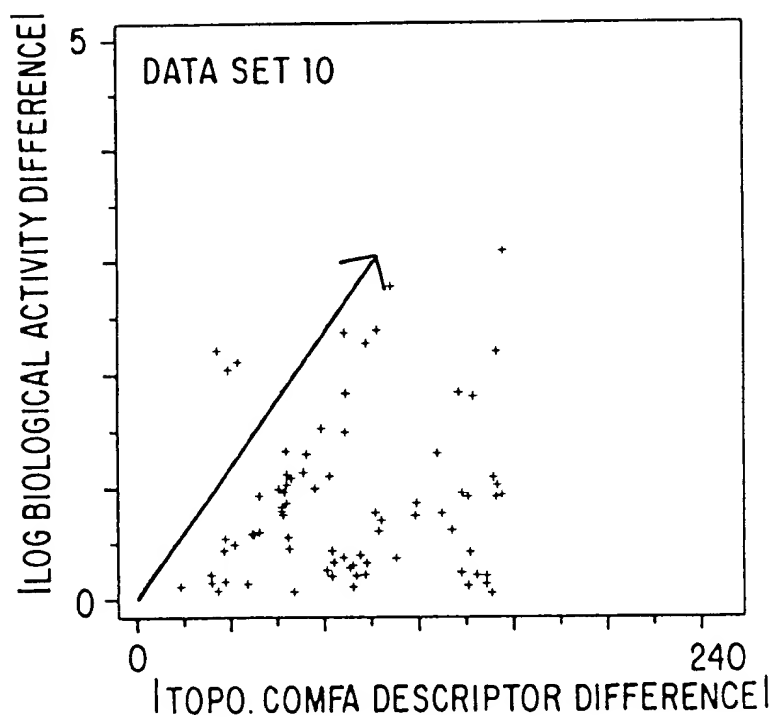


FIG.7(j)

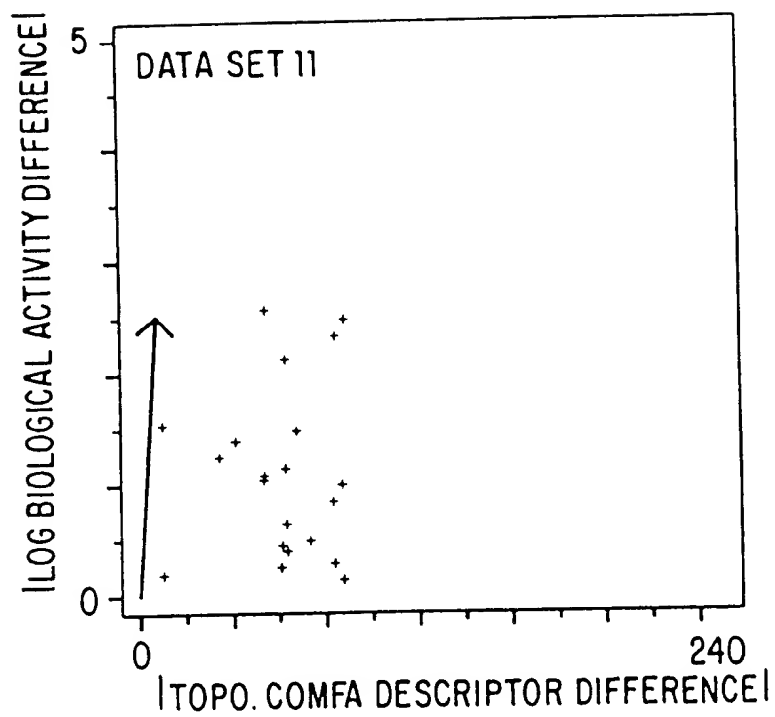


FIG.7(k)

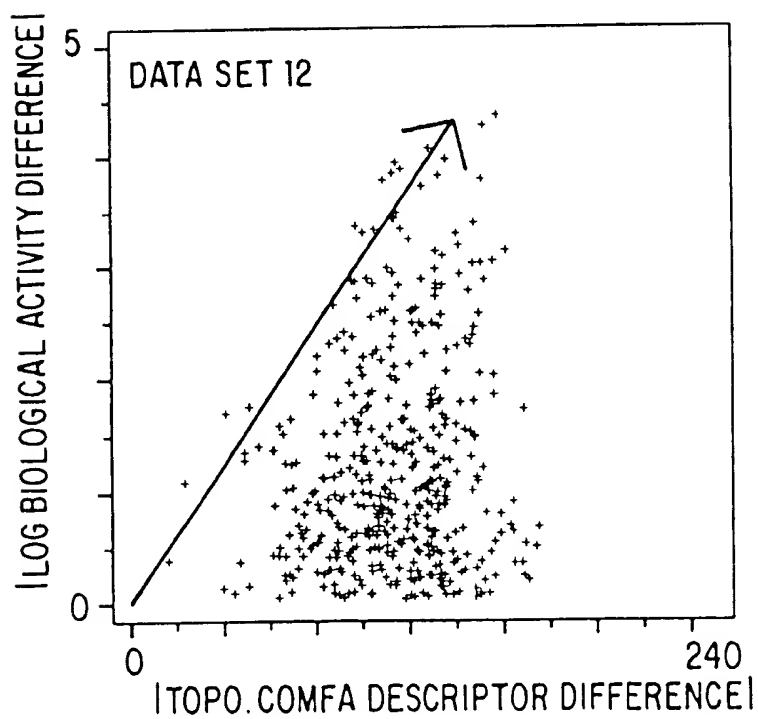


FIG.7(l)

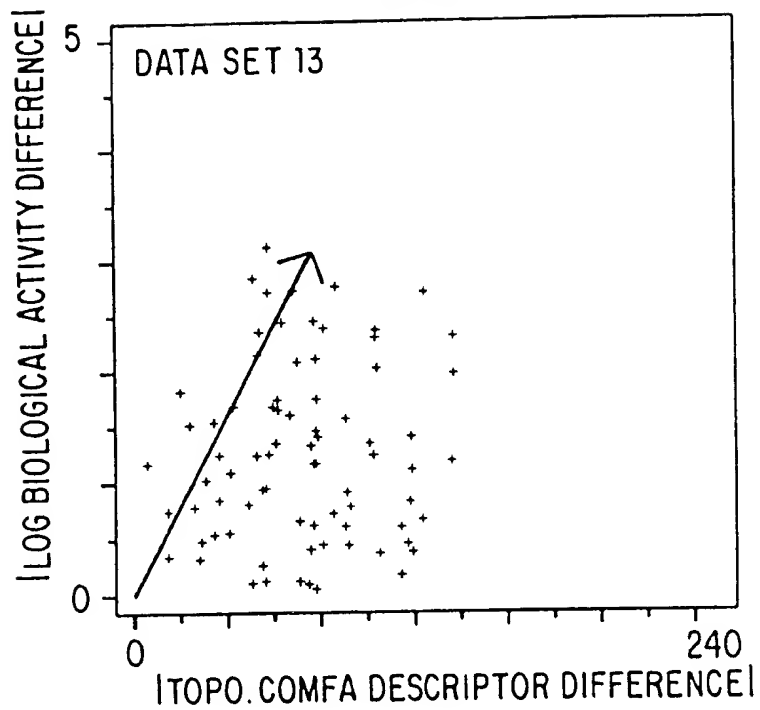


FIG.7(m)

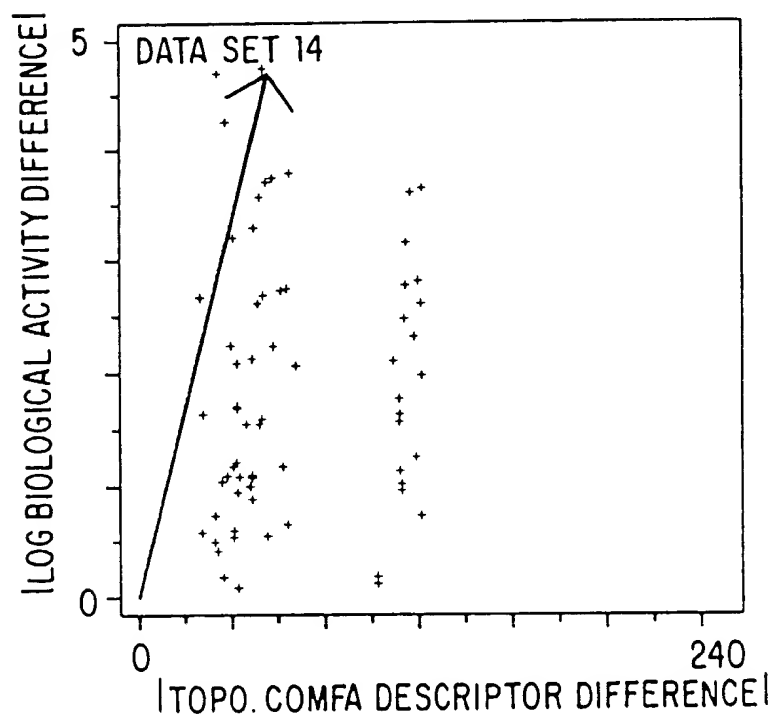


FIG.7(n)

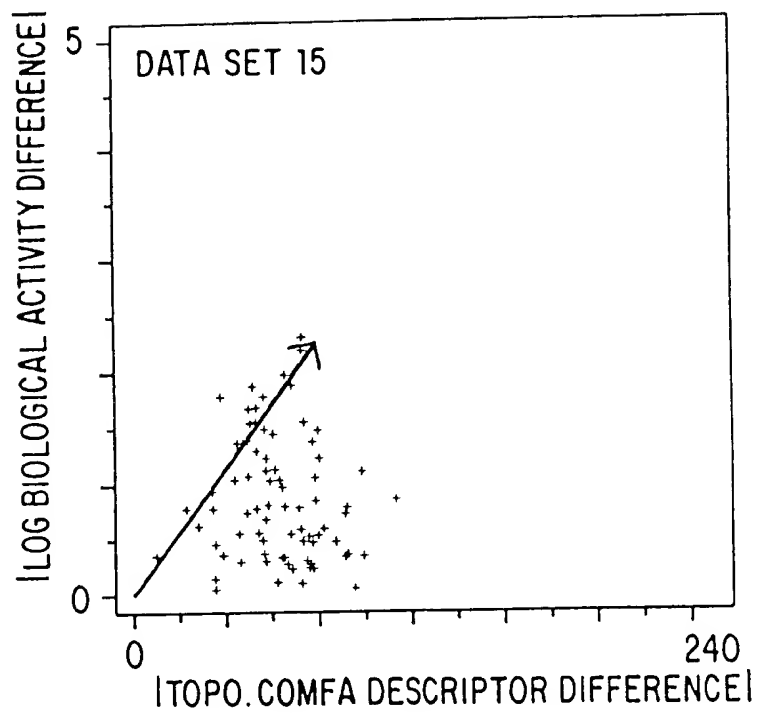


FIG.7(o)

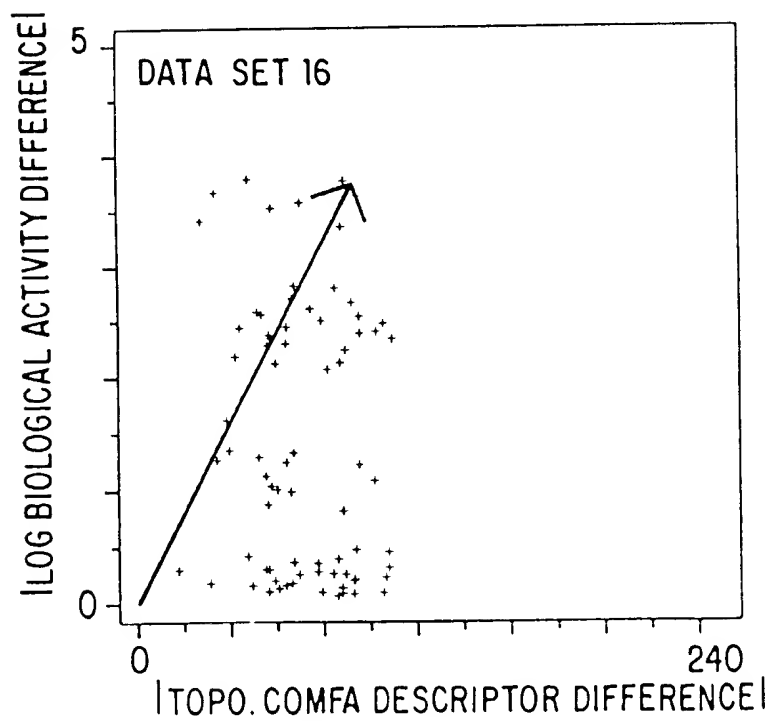


FIG.7(p)

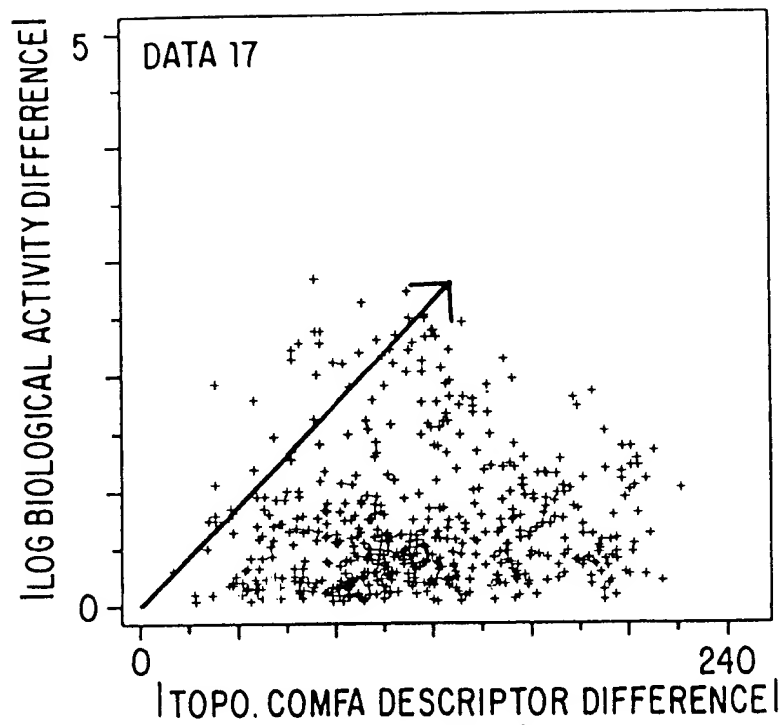


FIG.7(q)

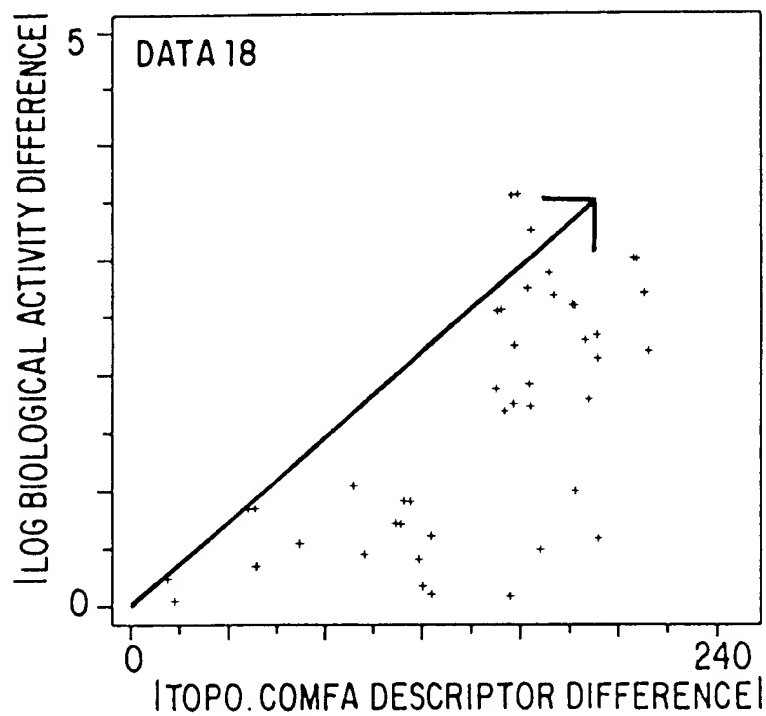


FIG.7(r)

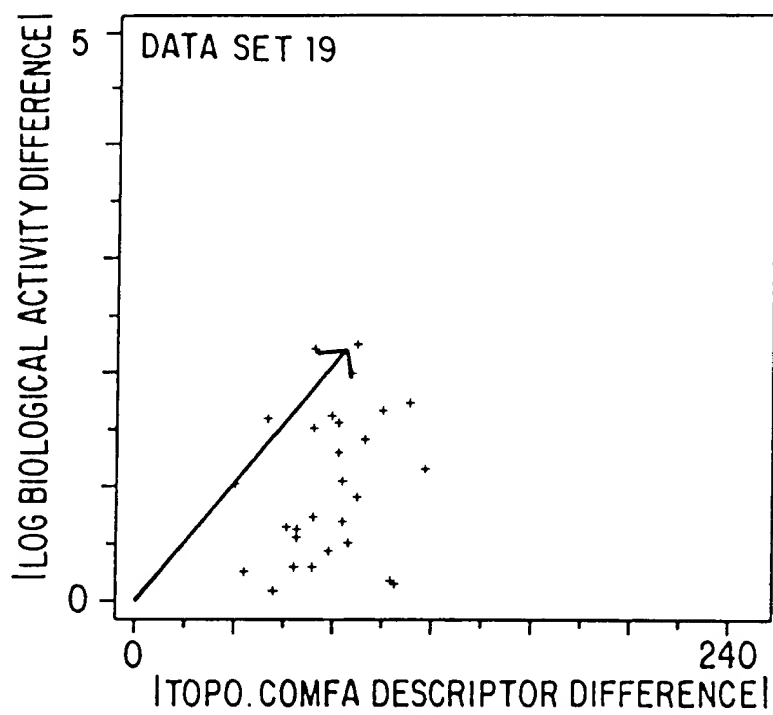


FIG. 7(s)

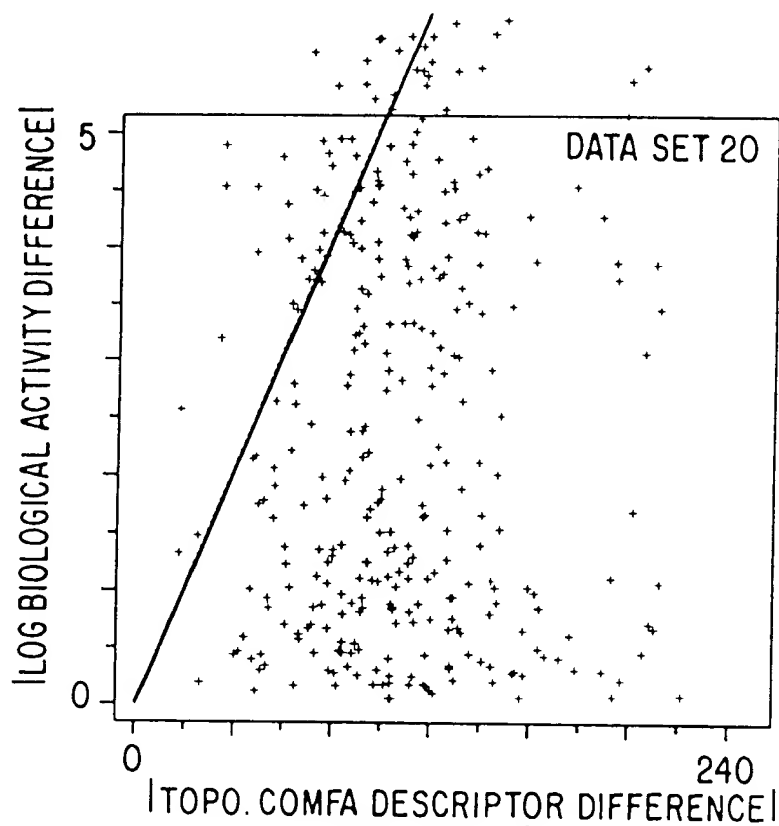
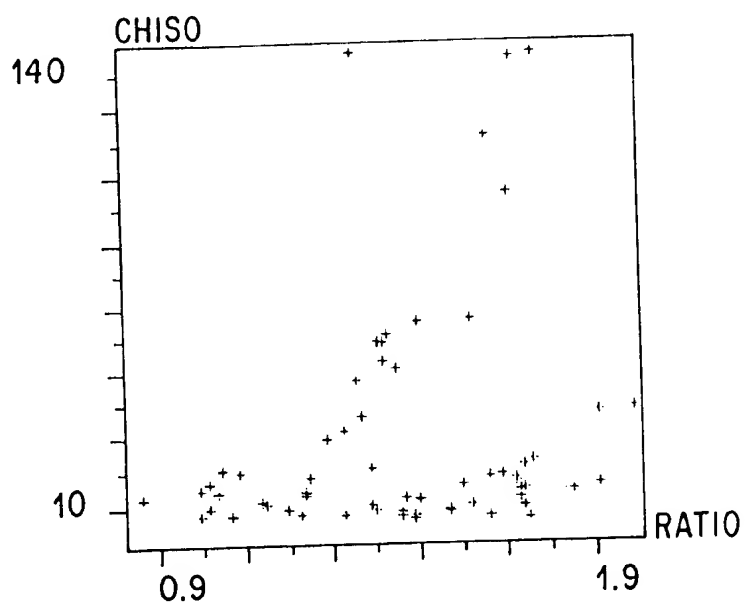


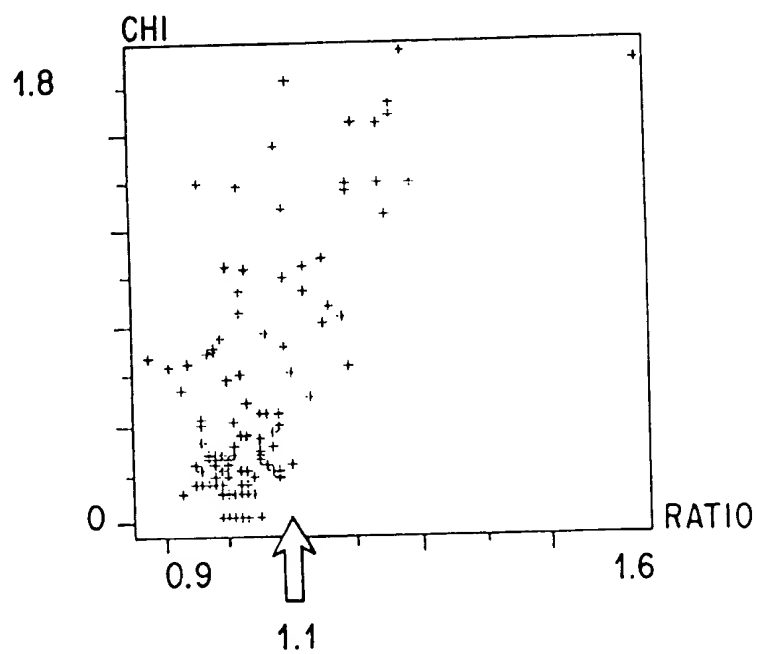
FIG. 7(t)

17/44



1.1

FIG. 8(a)



1.1

FIG. 8(b)

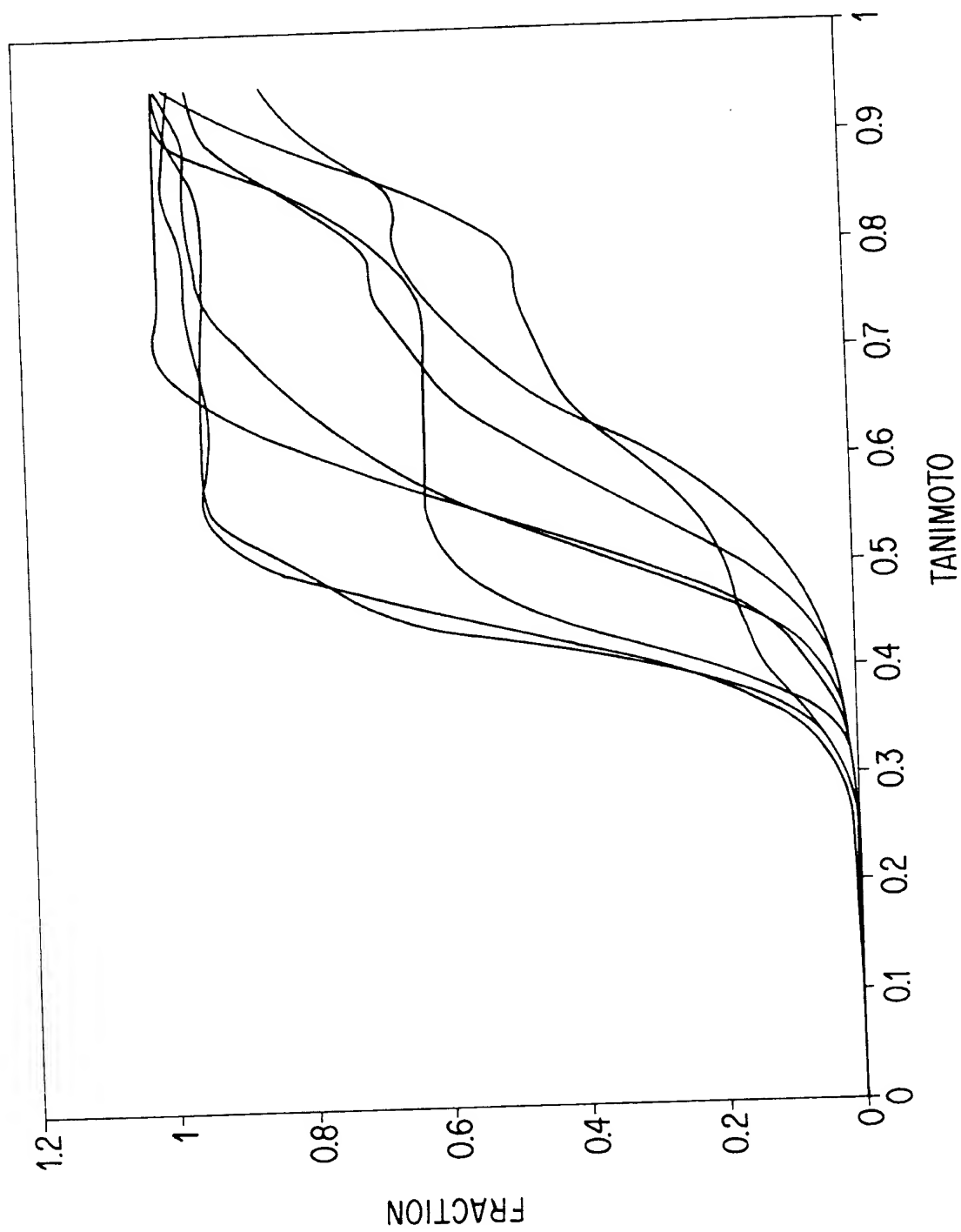


FIG. 9(a)

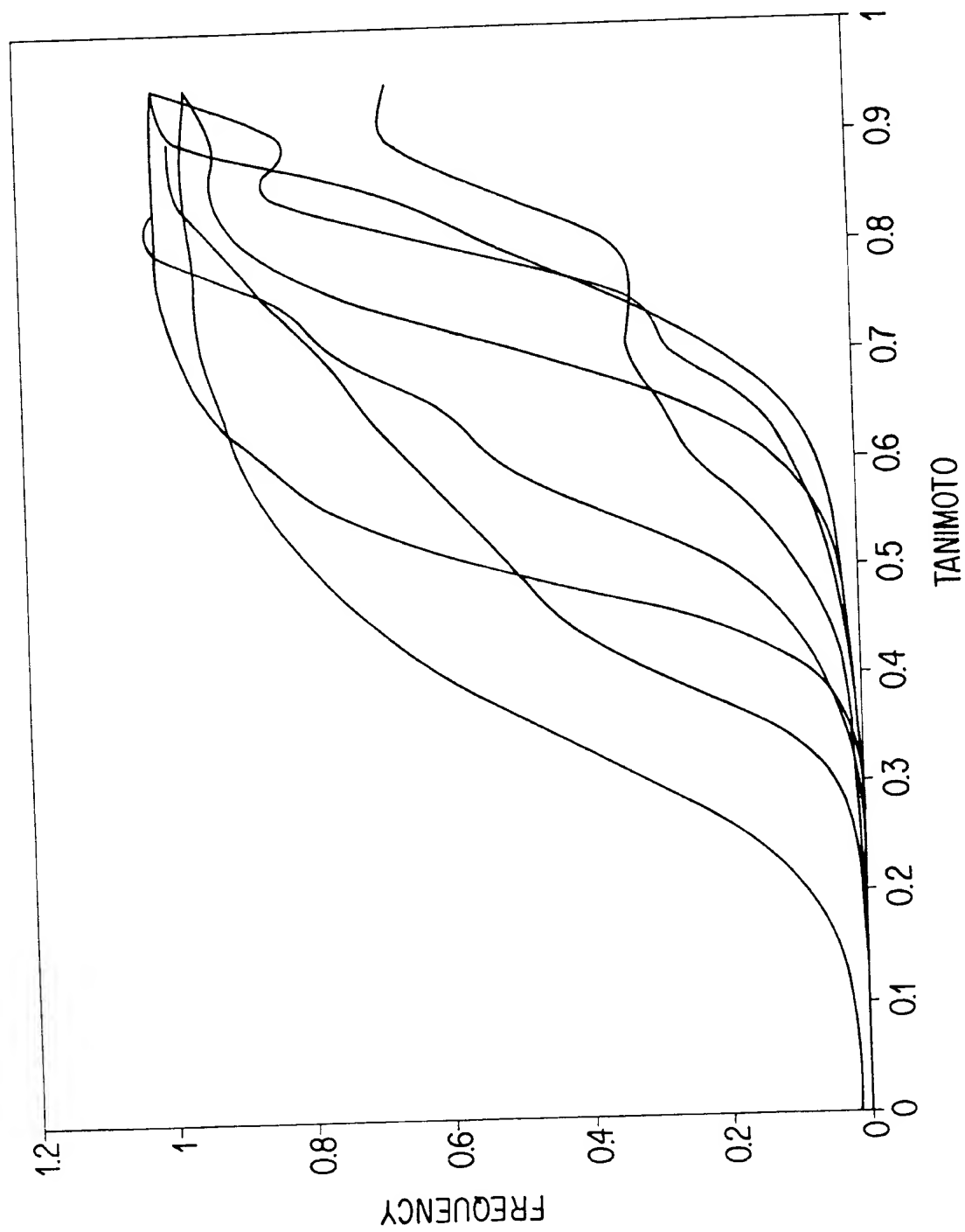
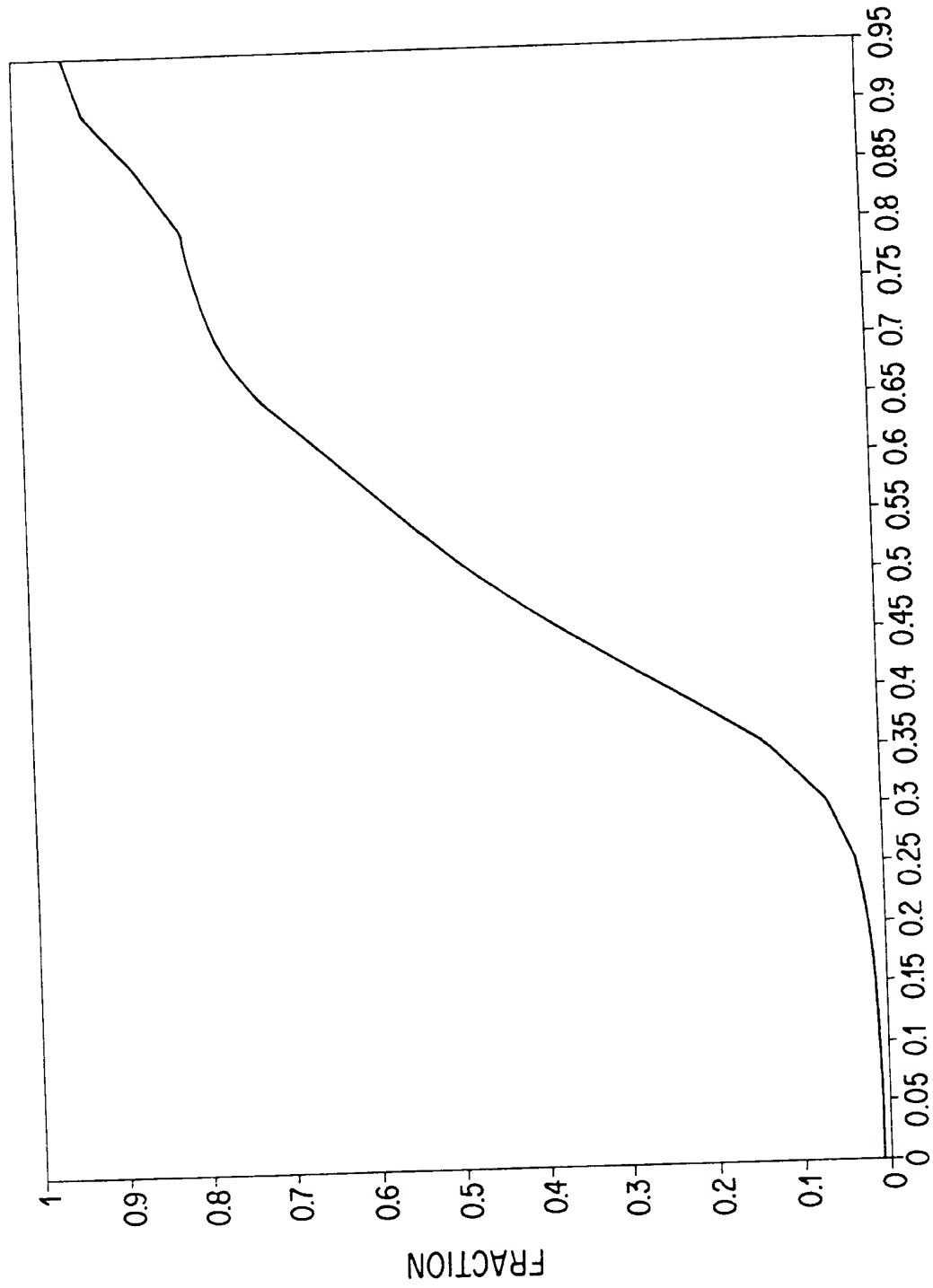


FIG. 9(b)



TANIMOTO

FIG. 9(c)

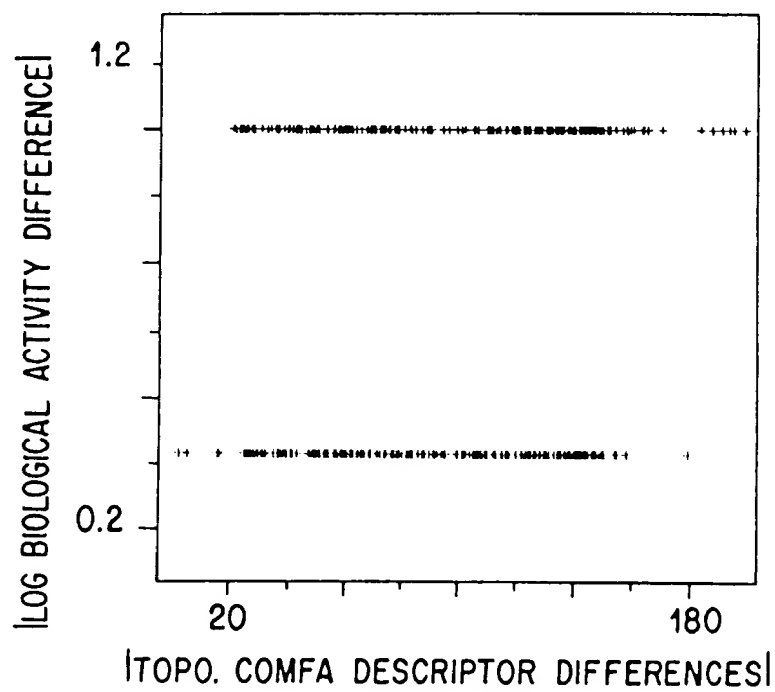


FIG.10(a)

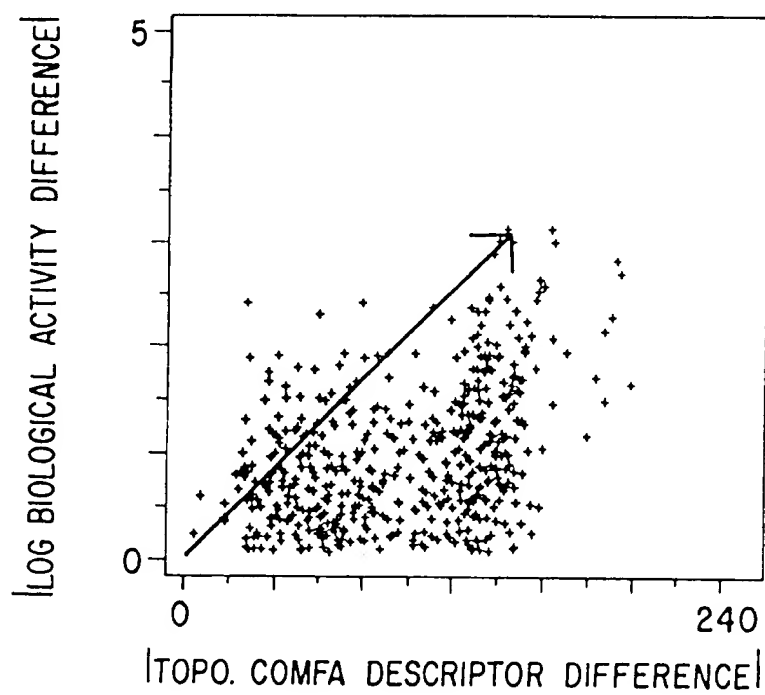


FIG.10(b)

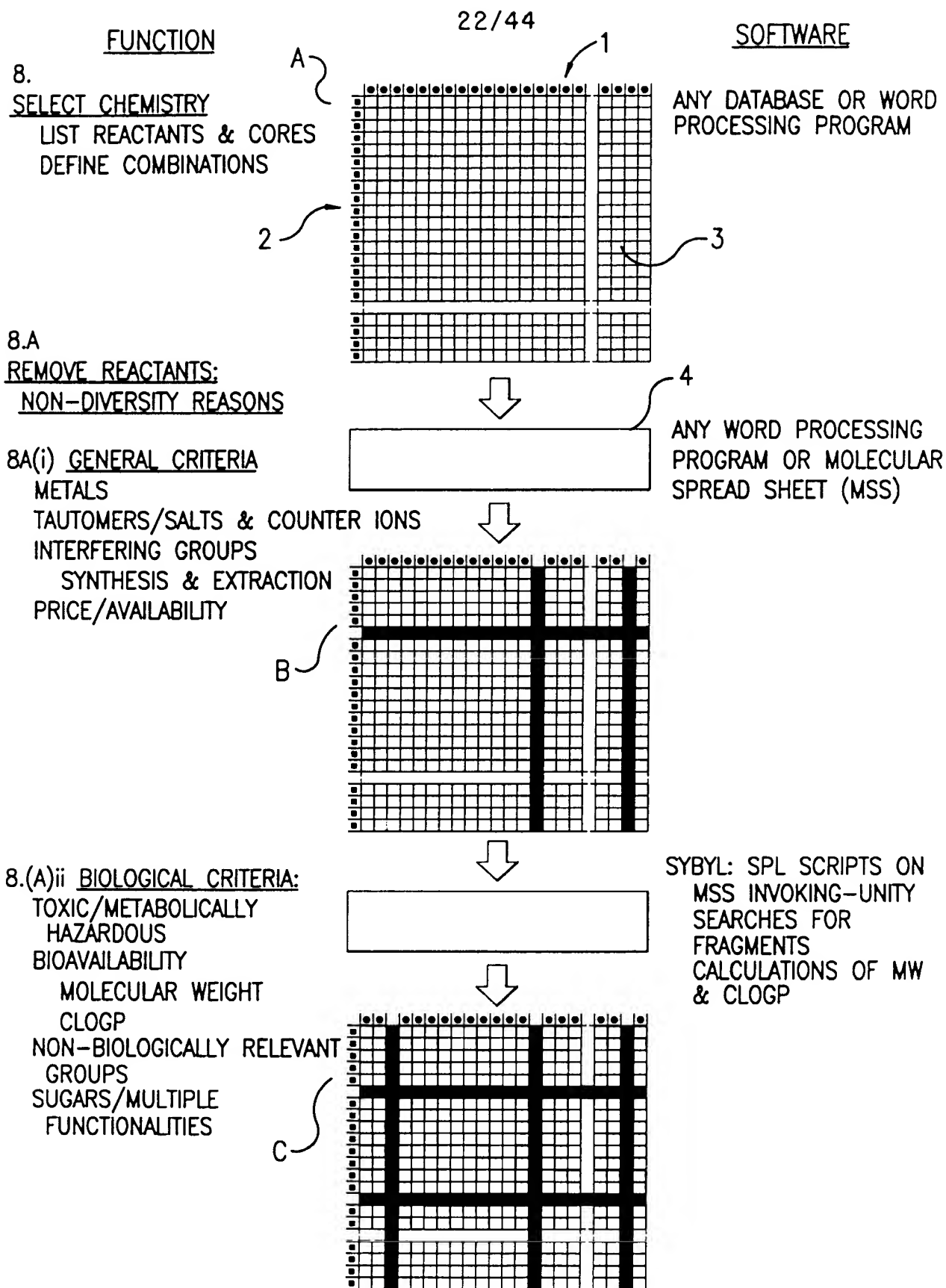


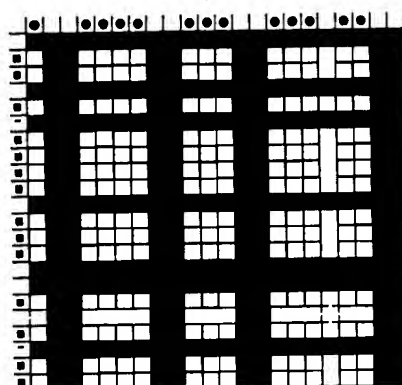
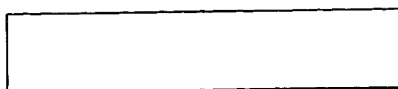
FIG.11(a)

8B

REMOVE NON-DIVERSE REACTANTS:

3D STRUCTURE GENERATION
 TOPOMERIC CONFORMER
 ALIGNMENT
 CoMFA FIELD GENERATION:
 HYDROGEN BOND FIELD
 GENERATION
 ROTATABLE BOND FIELD
 ATTENUATION
 CALCULATE FIELD
 DIFFERENCES
 CLUSTER
 REACTANT SELECTION FROM
 EACH CLUSTER

23/44



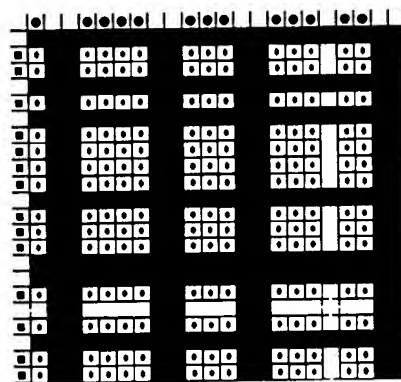
SYBYL: SELECTOR &
 CONCORD 3.2.1
 SPECIALIZED SOFTWARE:
 APPENDIX "A"
 (SYBYL: CoMFA
 STERIC & MSS)

SYBYL: HIERCHICAL
 CLUSTER - MSS
 SYLBL: MSS

8C

COMBINE REACTANTS TO BUILD PRODUCTS

E



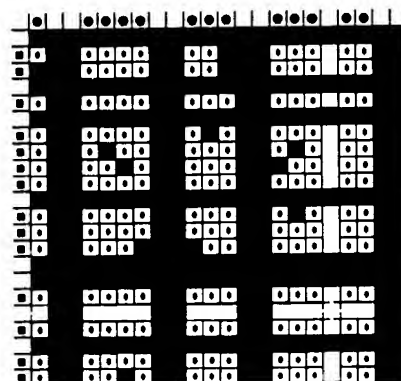
SYBYL: LEGION MSS

8D

REMOVE PRODUCTS:
NON-DIVERSITY REASONS

GENERAL CRITERIA:

F



SYBYL: SPL SCRIPTS
 ON MSS



FIG.11(b)

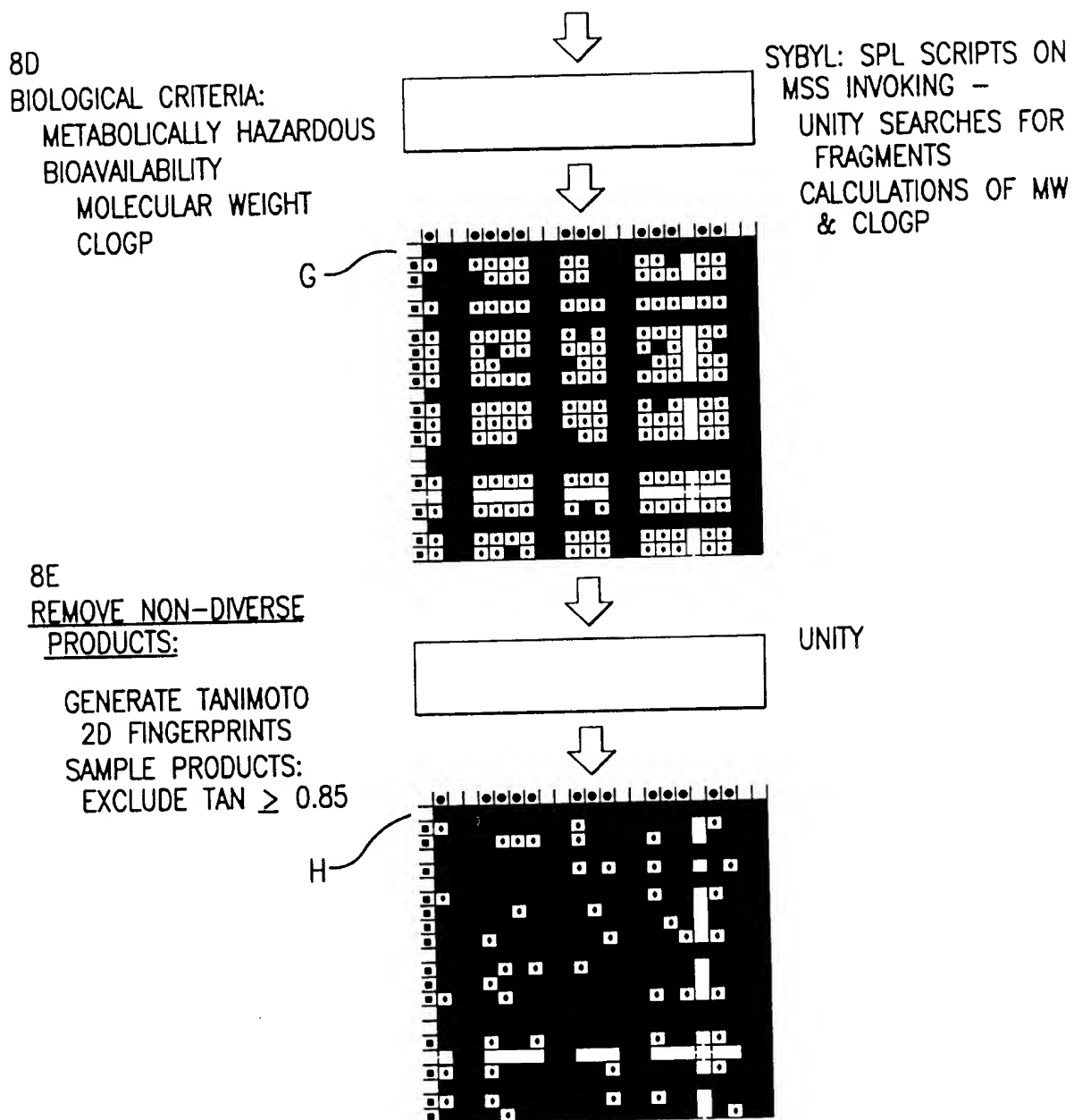


FIG.11(c)

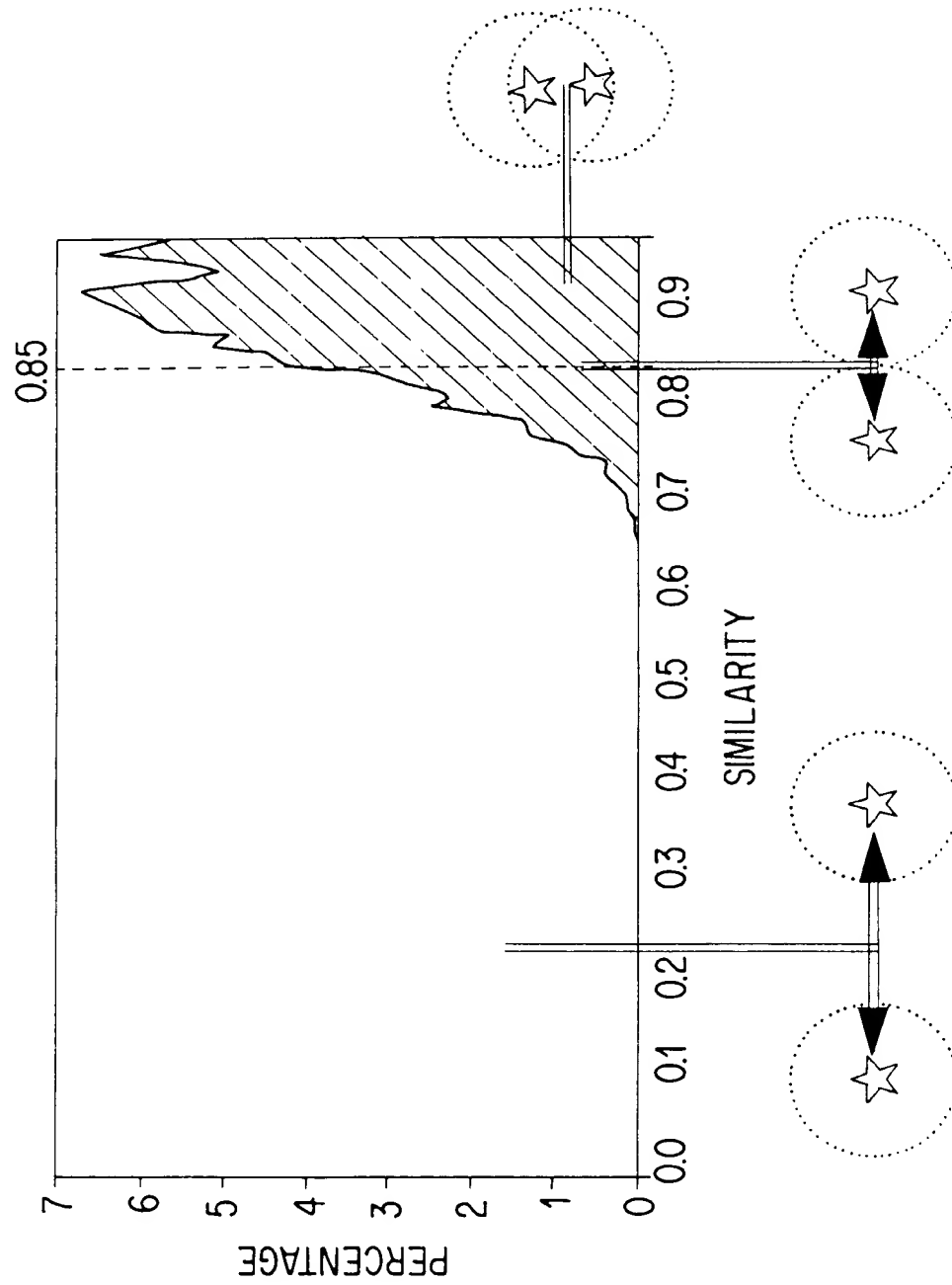


FIG. 13

27/44

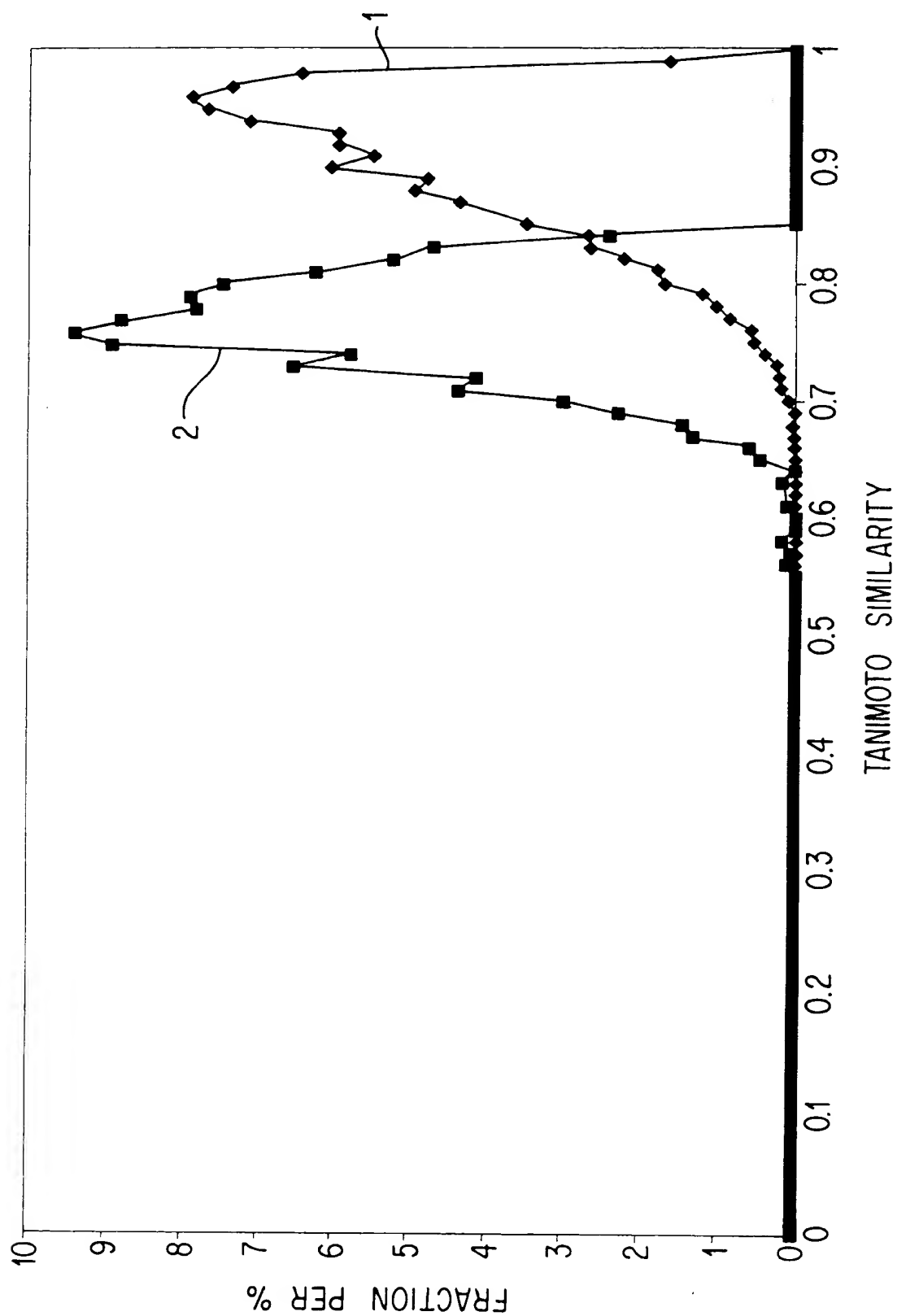


FIG. 14

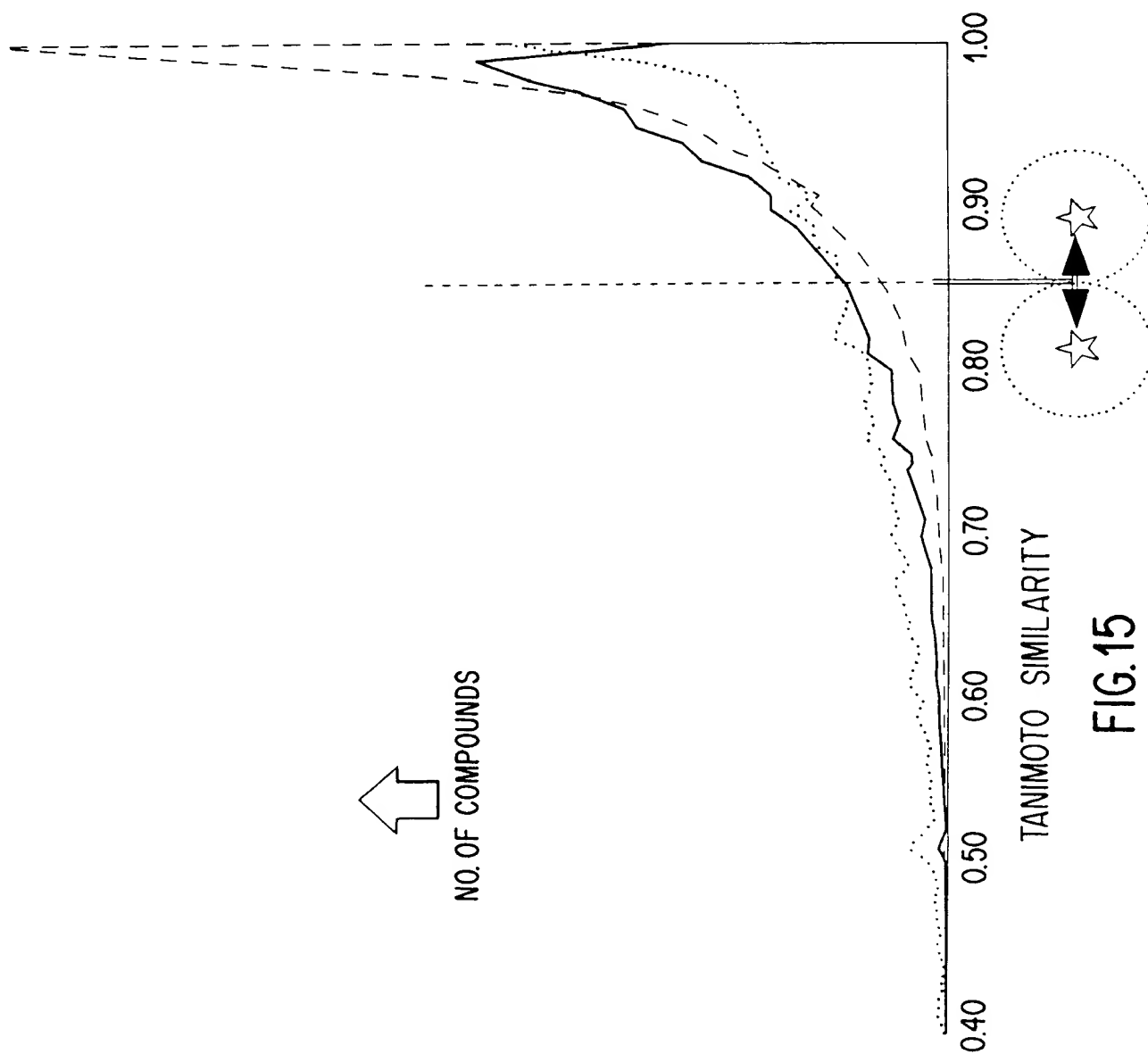


FIG. 15

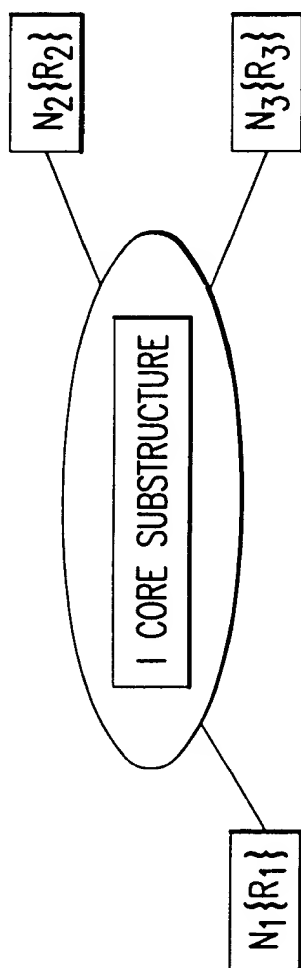


FIG.16

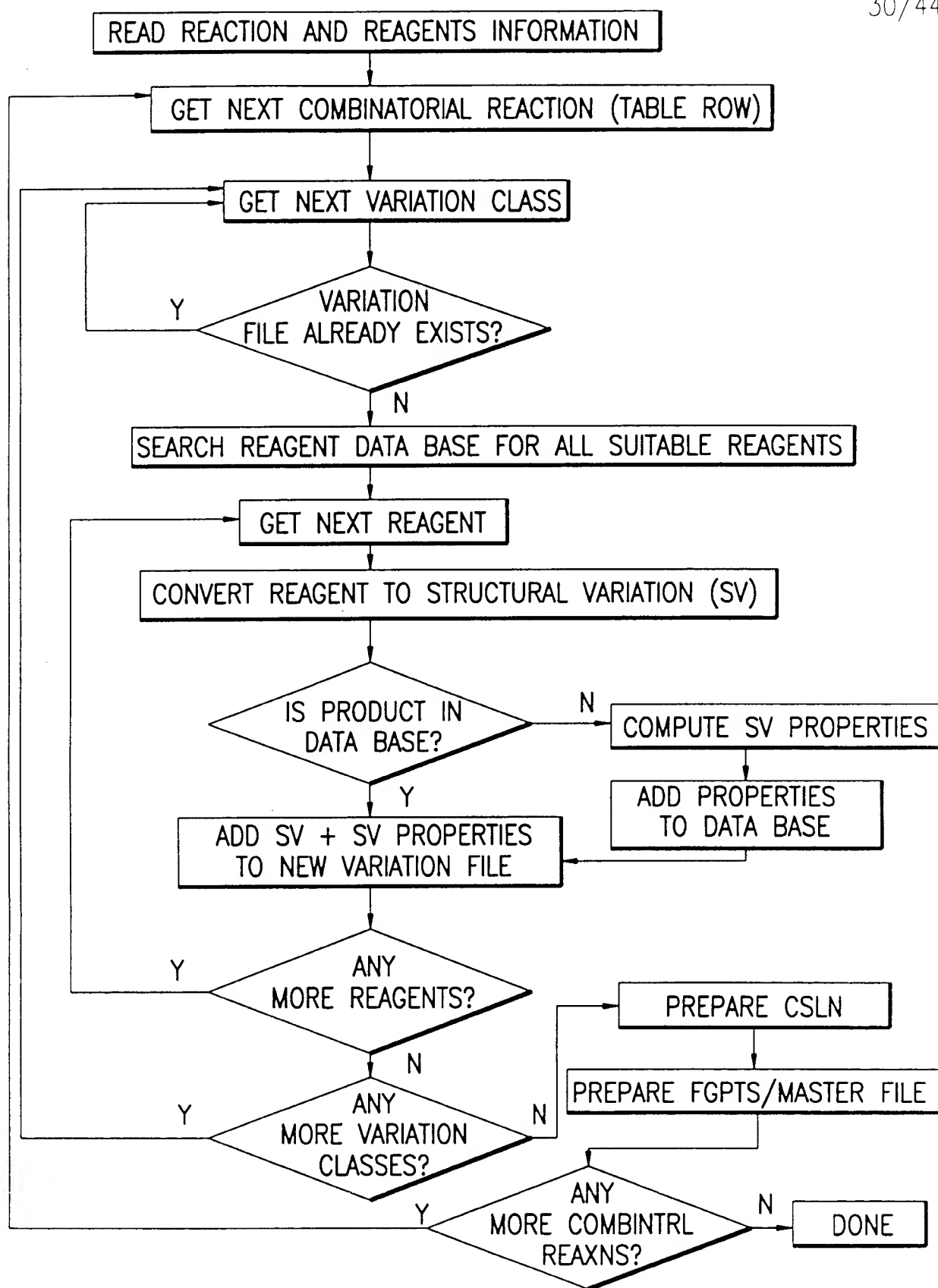


FIG.17

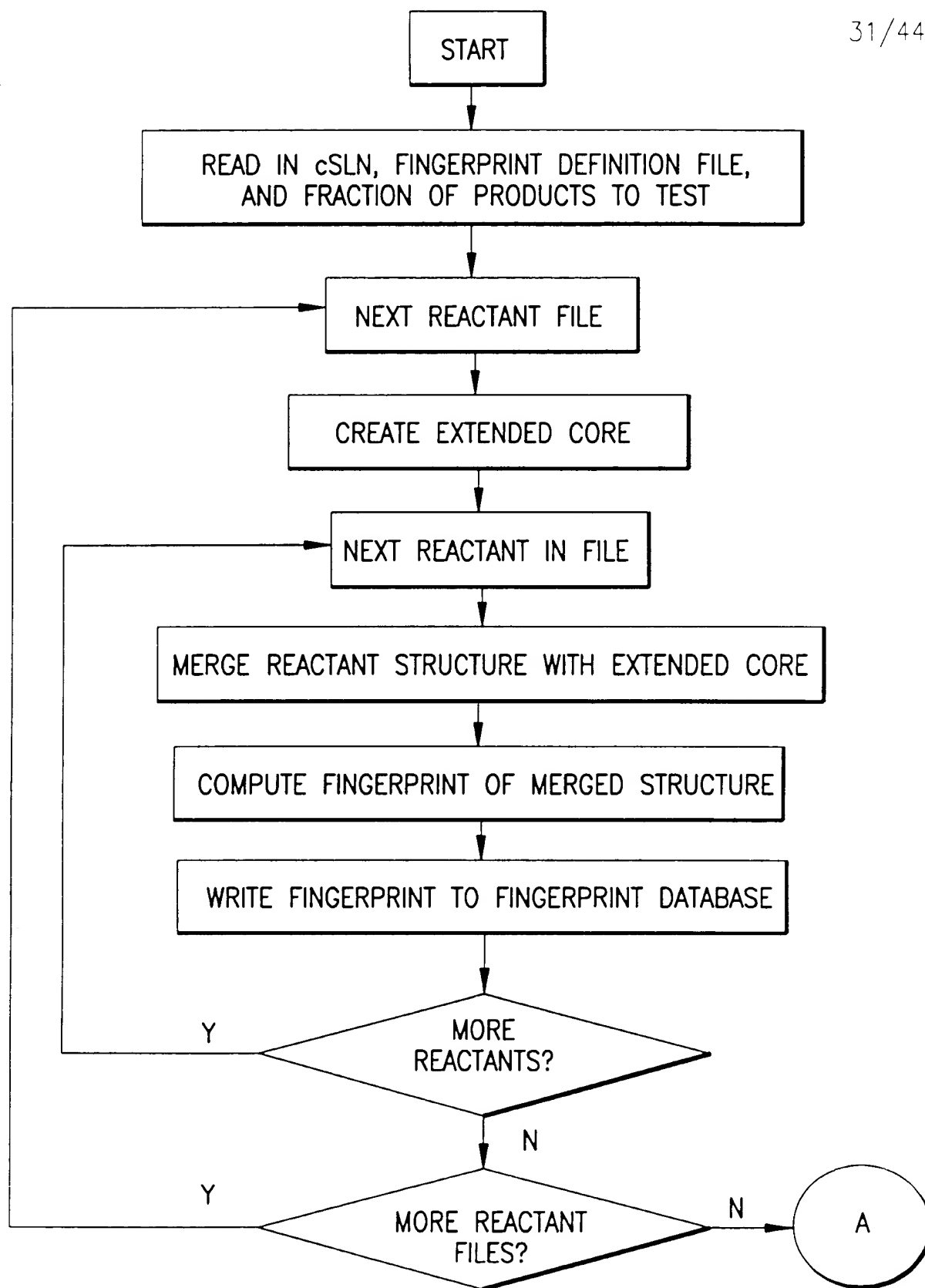


FIG.18

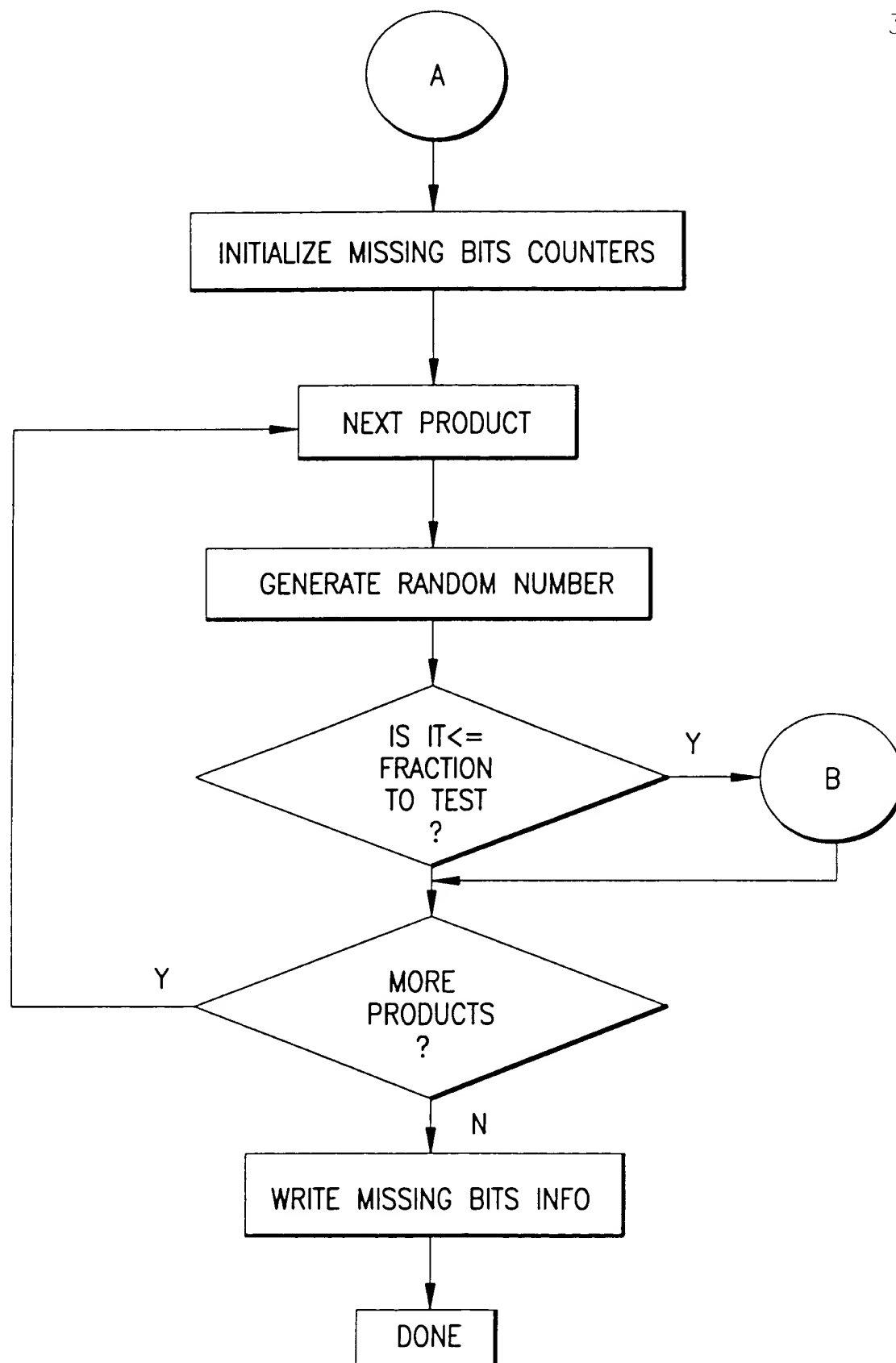


FIG.19

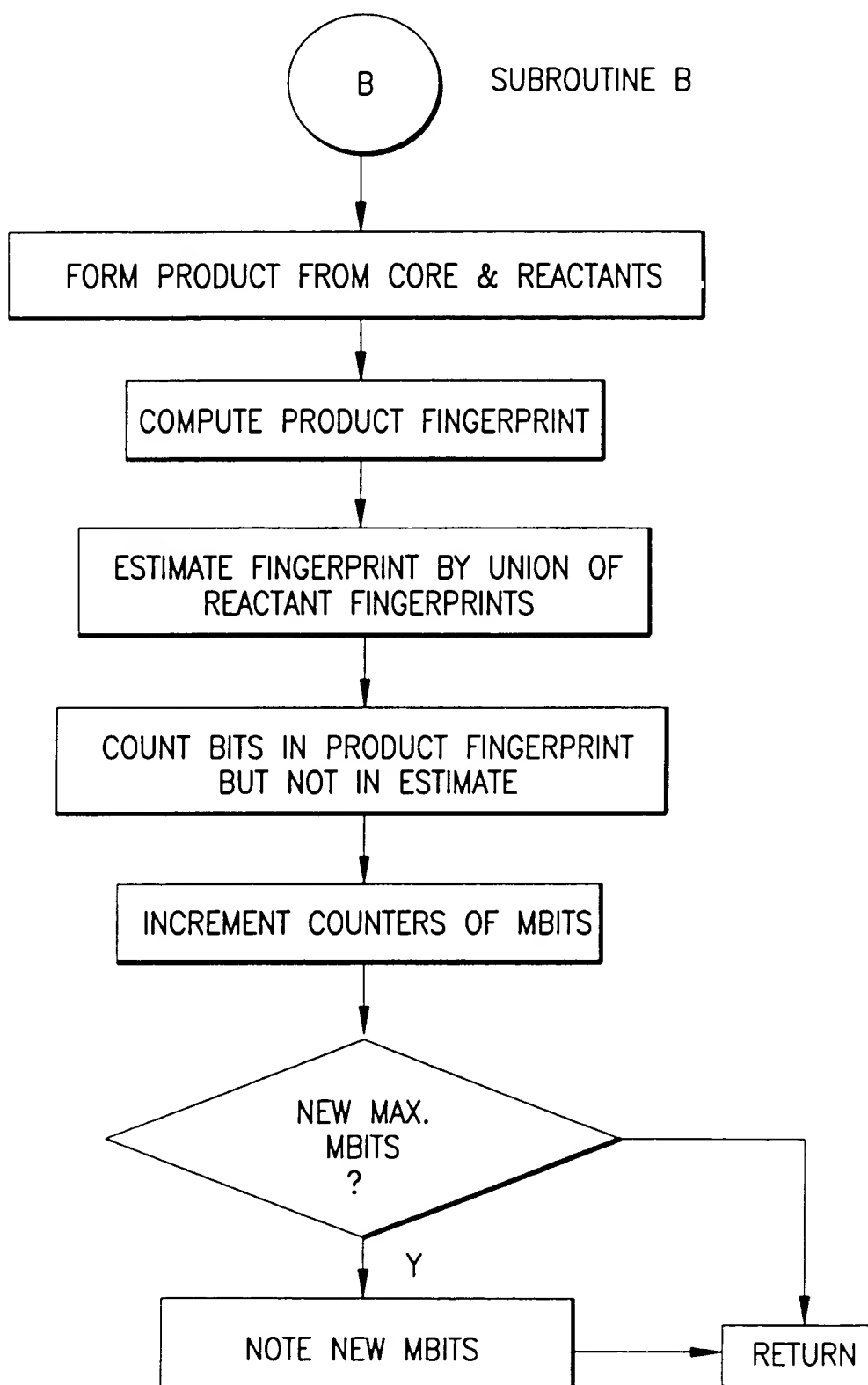


FIG.20

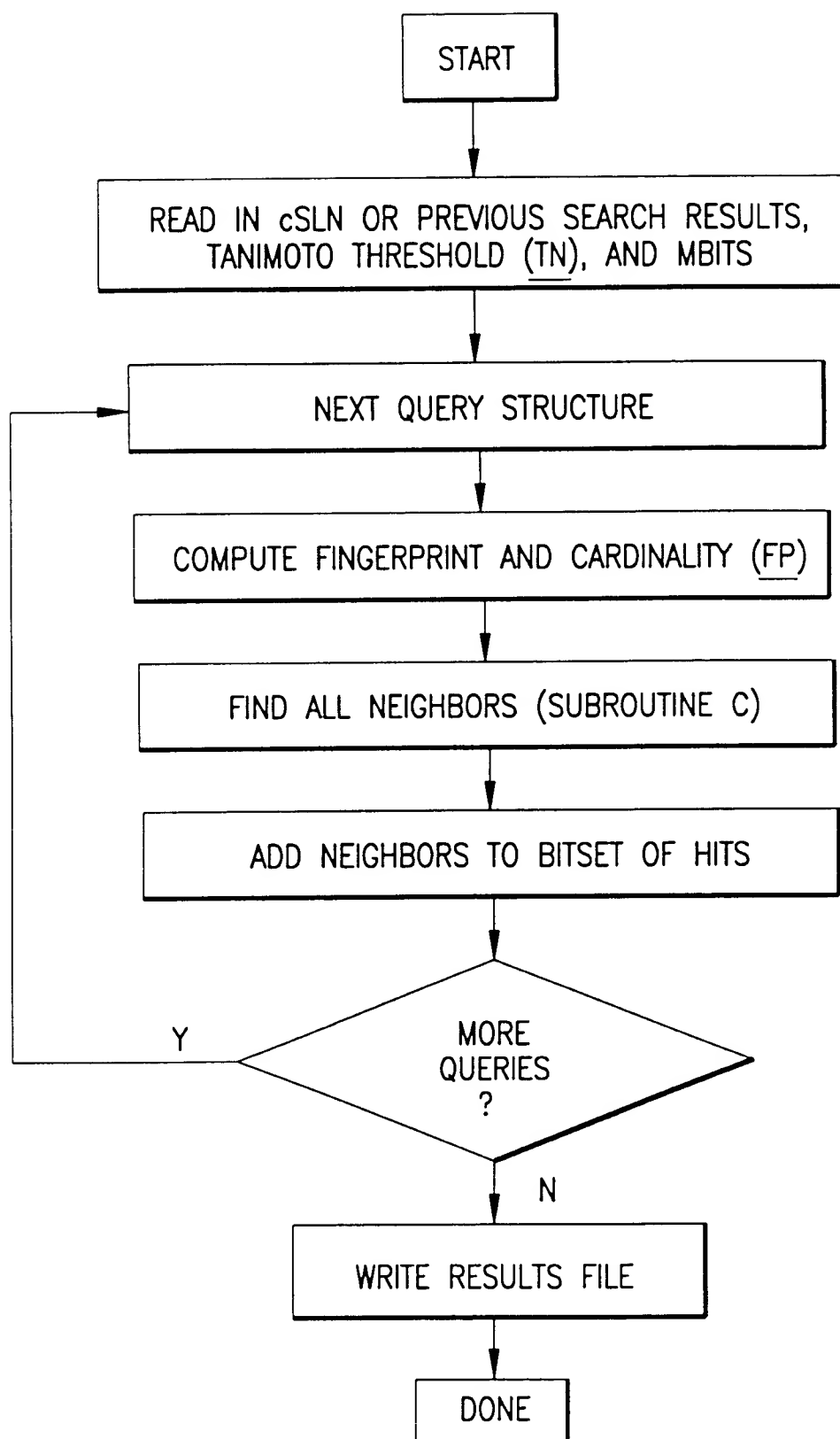
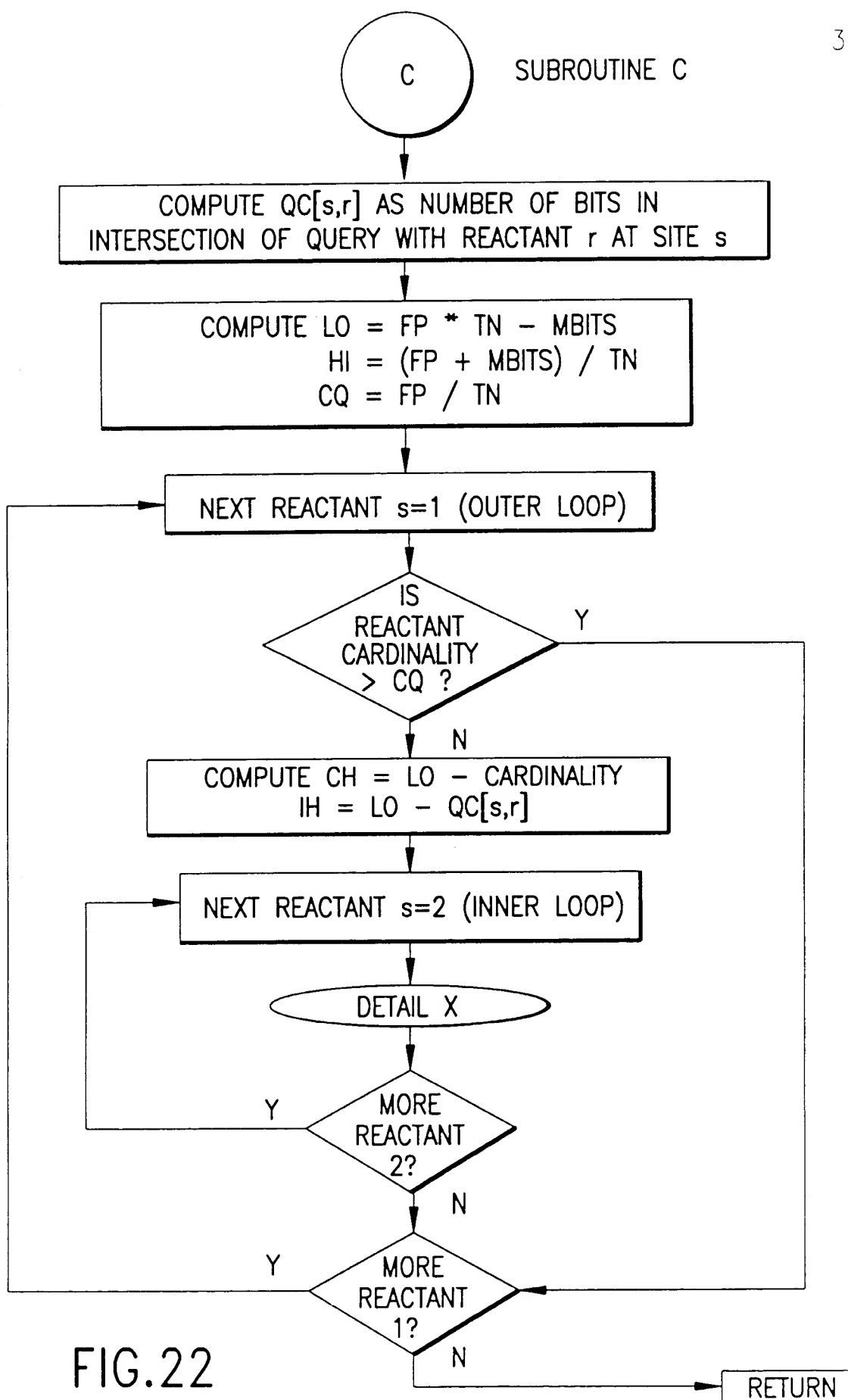


FIG.21



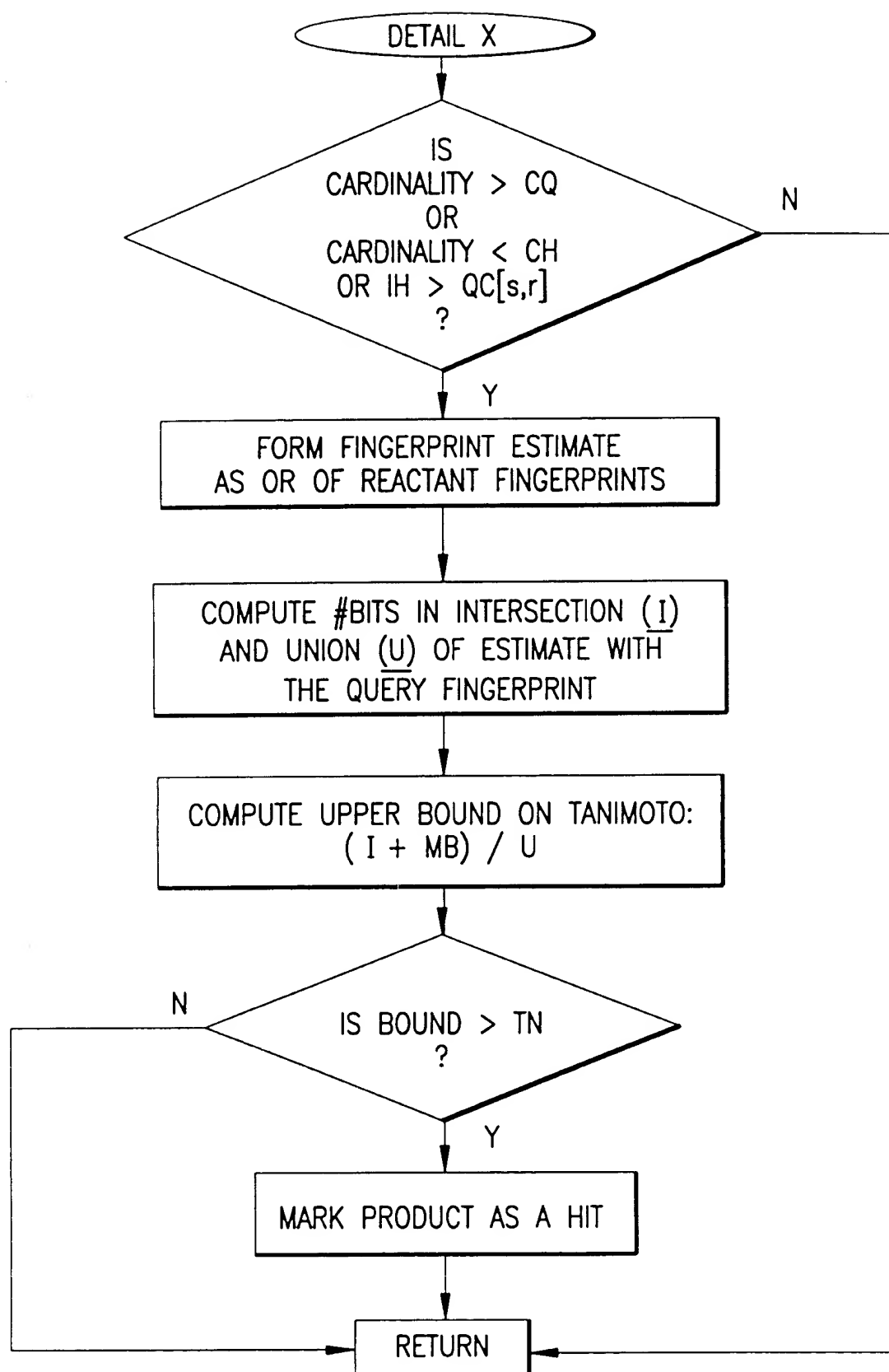


FIG.23

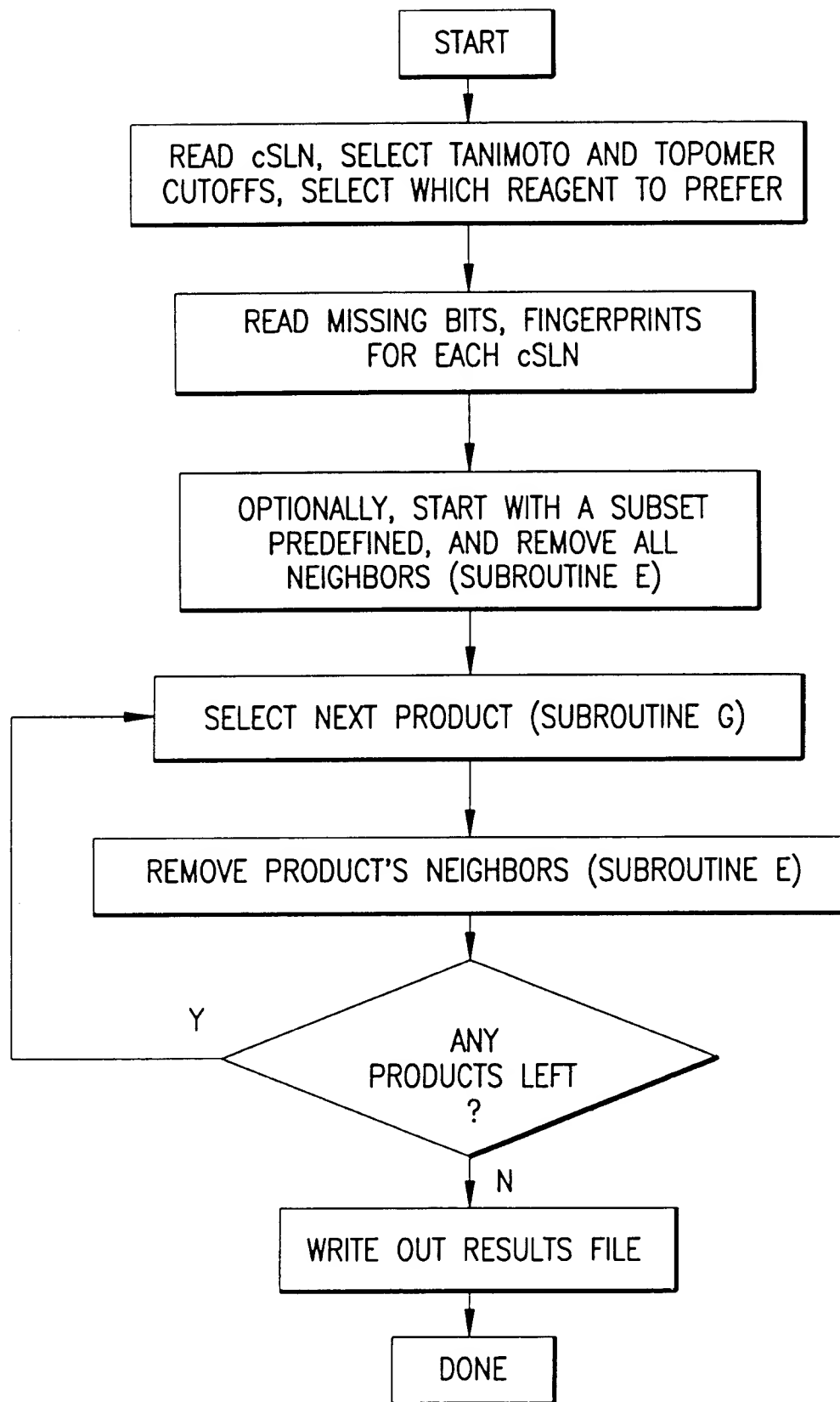


FIG.24

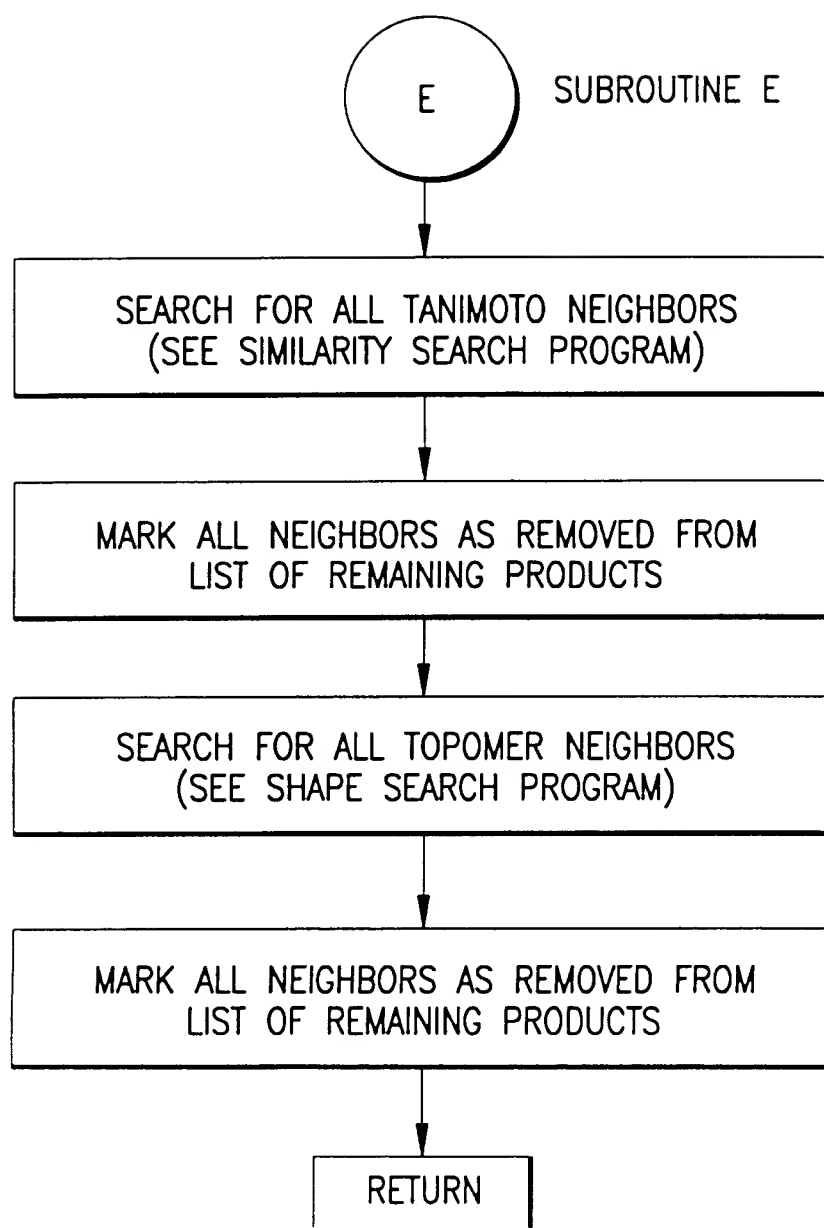


FIG.25

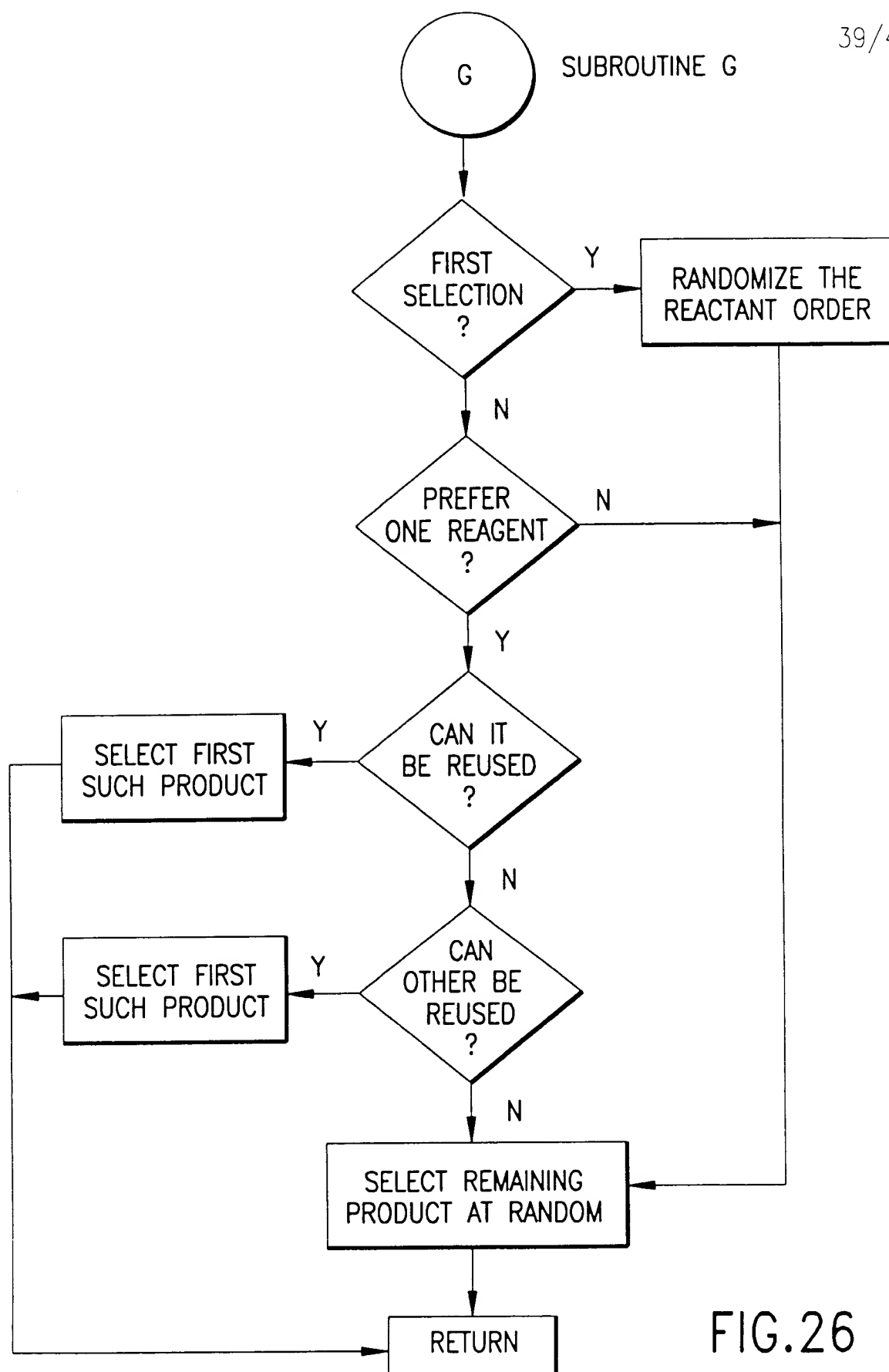


FIG.26

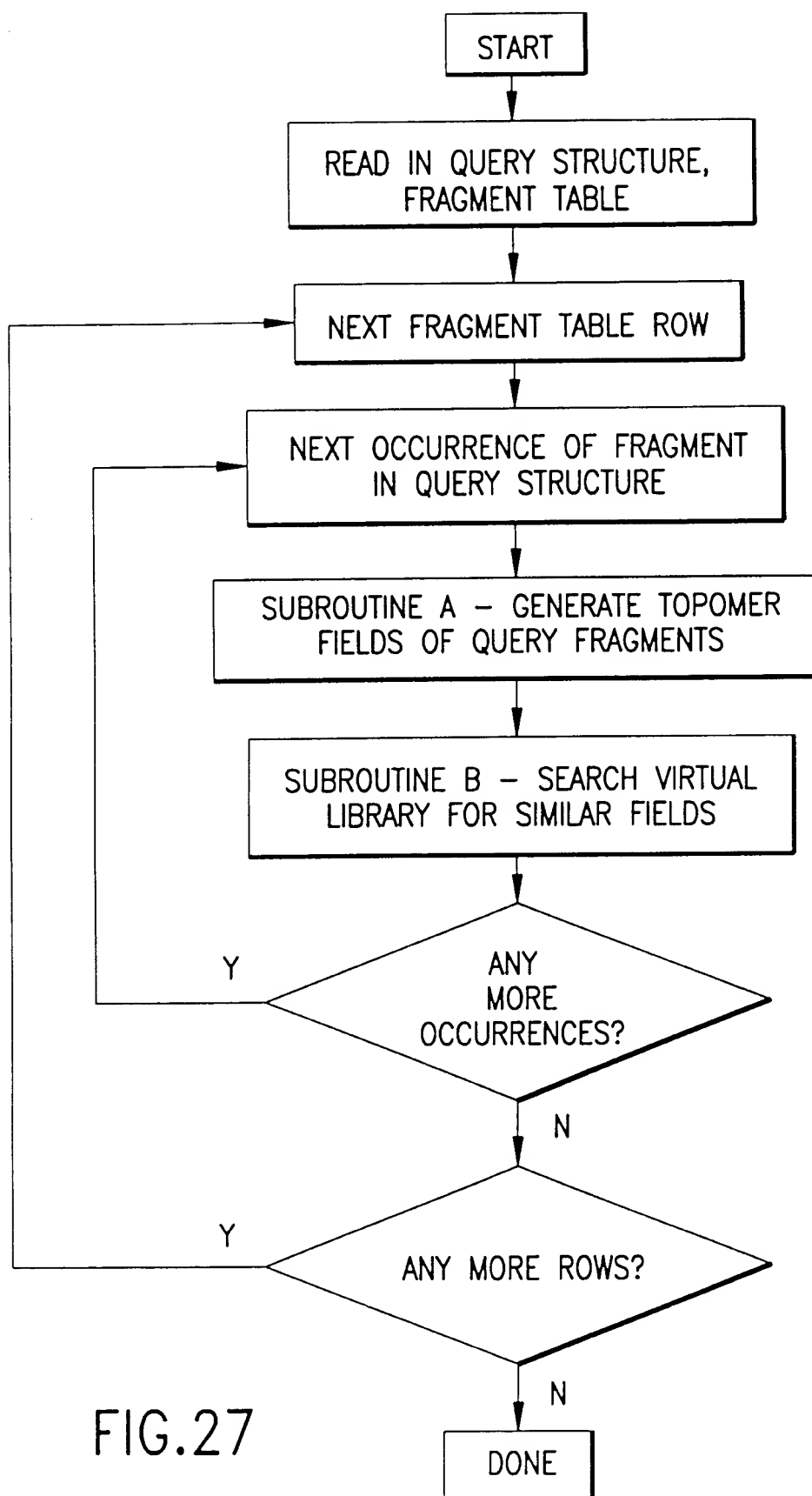


FIG.27

SUBROUTINE A

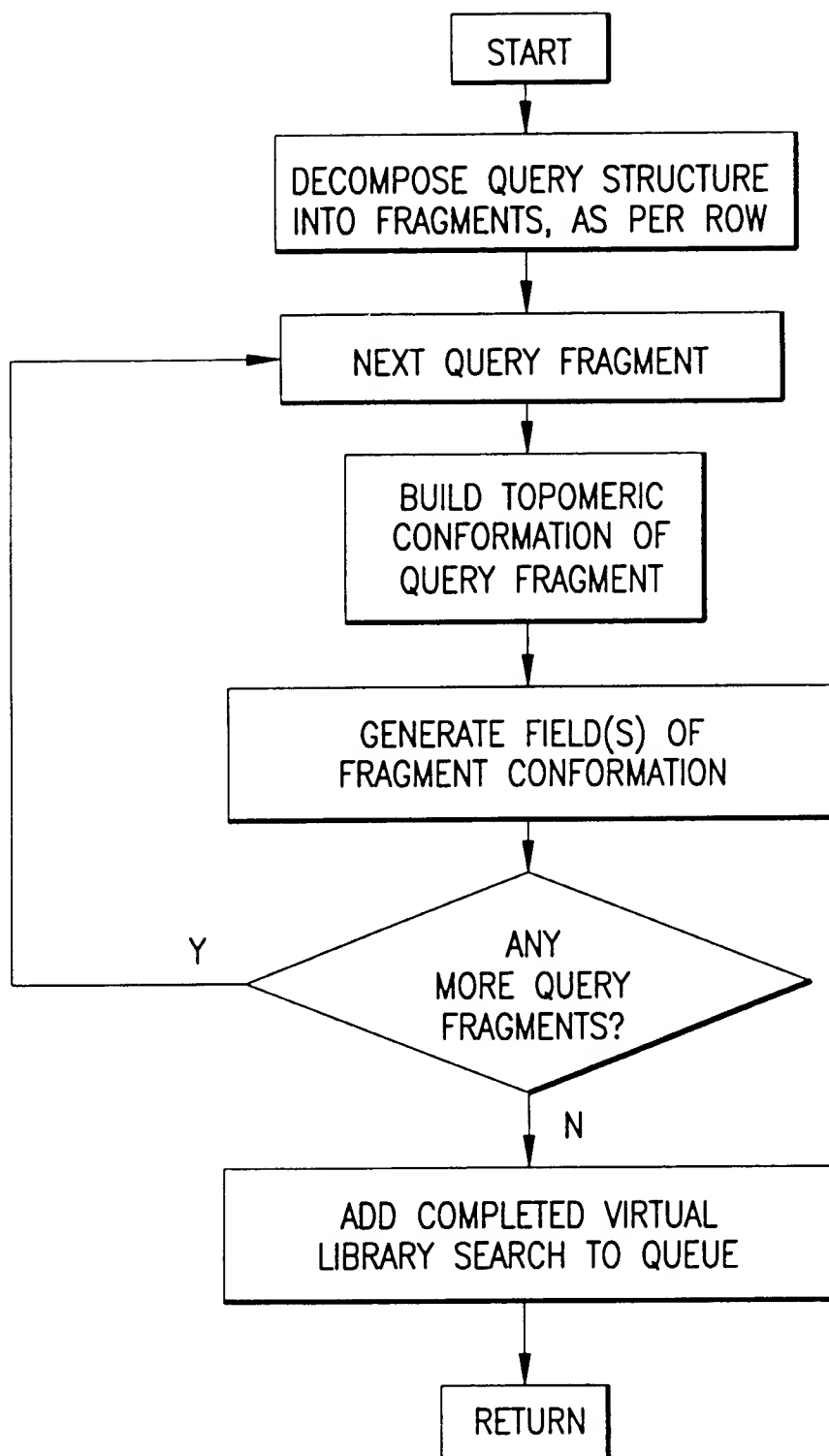
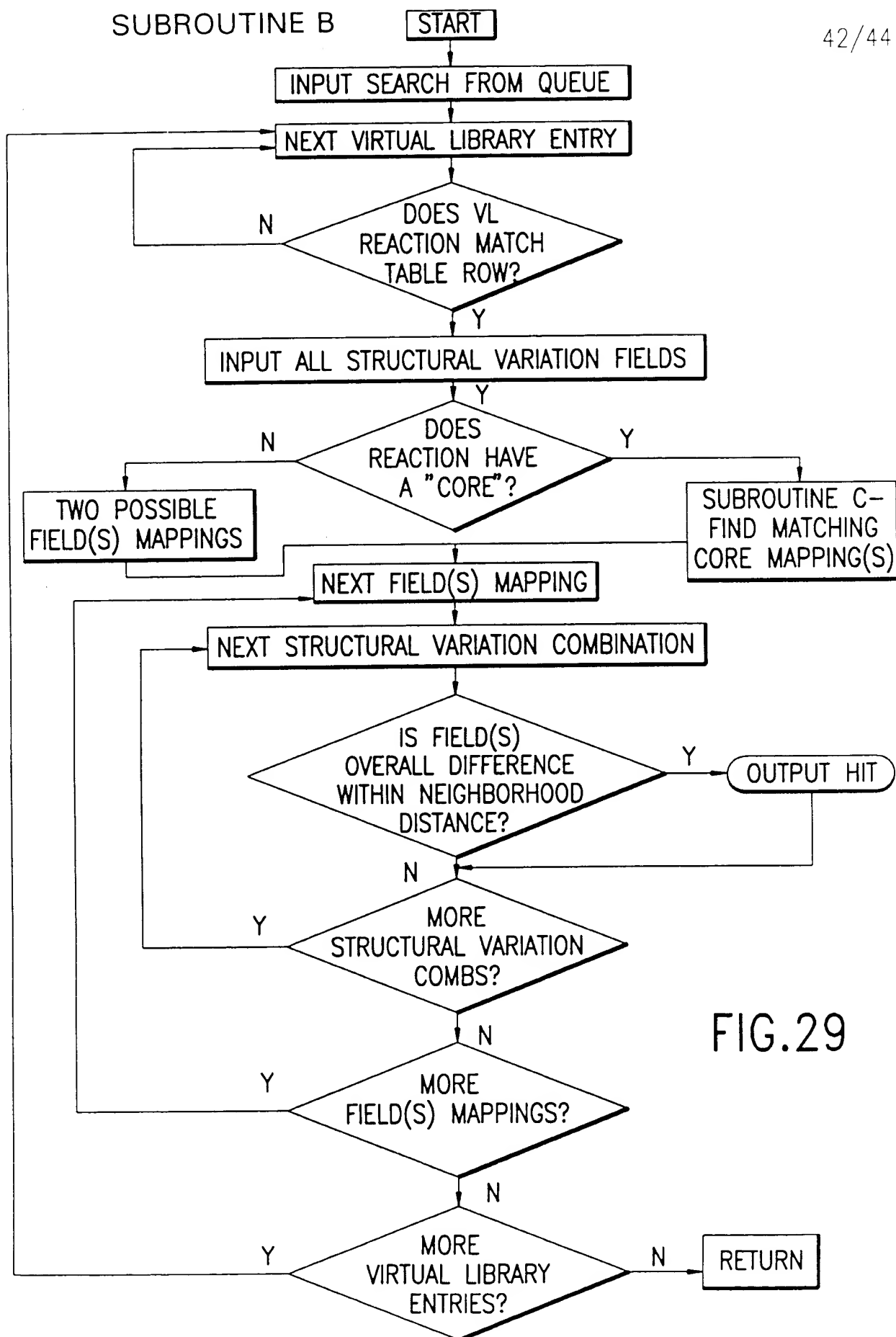


FIG.28



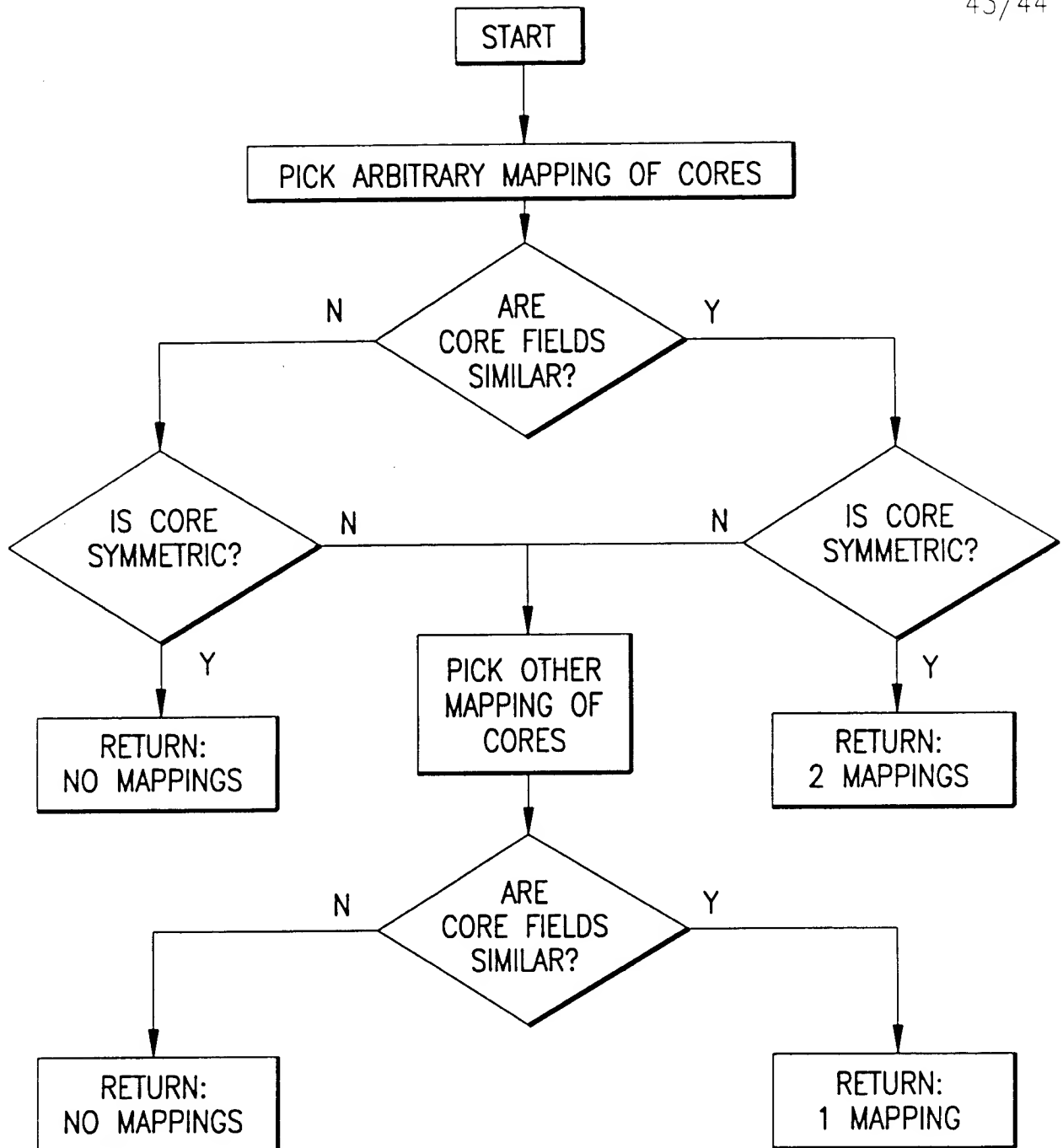


FIG.30

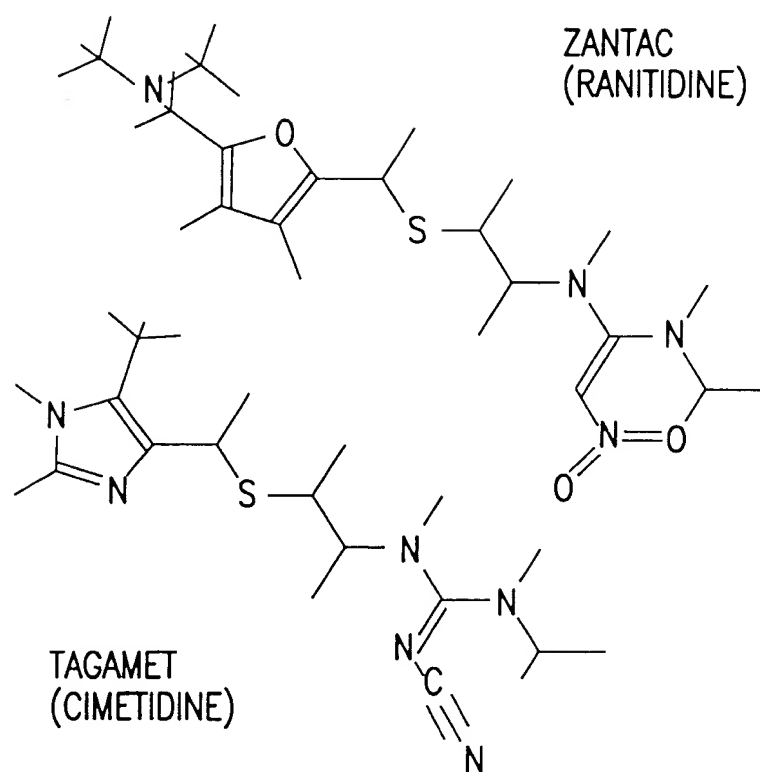


FIG.31